



Capability Portfolio Status Report

High End Computing Capability

April 10, 2019

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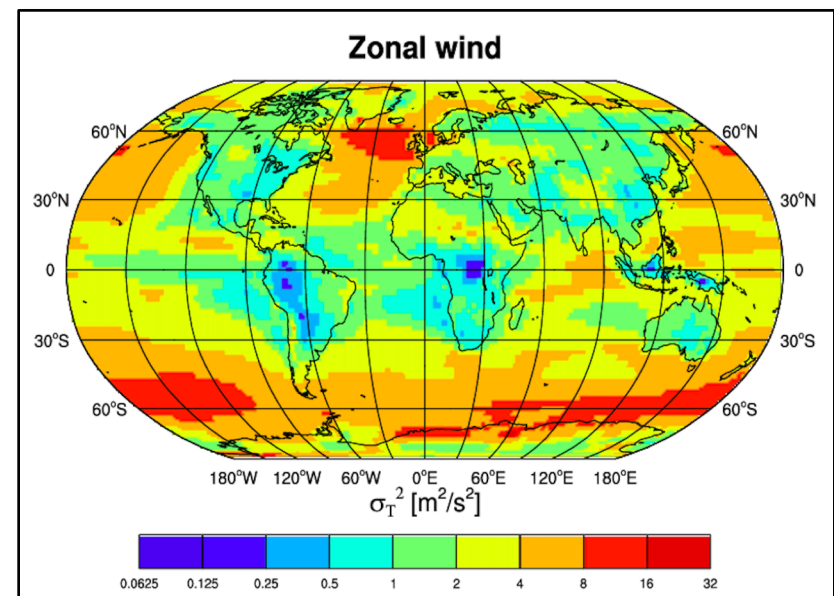
Applications Experts Improve GEOSgcm Job Efficiency by 25%



- HECC Application Performance and Productivity (APP) experts performed an in-depth analysis of the memory requirements to run the Goddard Earth Observing System-5 (GEOS-5) General Circulation Model, and found an efficient method of packing the processes that required 25% fewer Pleiades nodes.
 - The model run by user Ehud Strobach required 7,776 processes. His jobs previously used 432 Haswell nodes with only 18 processes per node. He was leaving 6 cores per node idle because using all 24 cores on each Haswell node would cause his job to run out of memory.
- The APP analysis of the memory requirements showed that:
 - The first process uses 32 GB of memory, and every 18th process uses 11 GB, with the rest of the processes using 4.4 GB each. A simple calculation showed that only the first node needs to leave 6 cores idle.
 - All the other nodes can run fully-populated with 24 processes, thus reducing the total number of nodes from 432 to 325—a savings of 25%.
- Each run takes 24 hours, so a 25% reduction in the number of nodes translates to a savings of over 2,000 SBUs* per run.

* 1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.

Mission Impact: Increasing the efficiency of large multi-node jobs saves usage allocations for an individual researcher, and also increases the pool of available resources for other users.



Climate models are the main tools used to simulate future climate conditions. However, the predictions made by these models are still subject to large uncertainties, and many computational runs with varying initial conditions are required to gauge the sensitivity of climate predictions to various model inputs.

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Remote Transfer Performance of Very Large Dataset Improved by Factor of 20



- Systems staff supported scientists at NASA's Langley Research Center to allow HECC's in-house Shift tool to better optimize the transfer of a 1-petabyte (PB) dataset from Oak Ridge National Lab (ORNL) to the NAS facility for additional processing.
- Initially, using the default settings of the Shift tool, transfers only achieved around 55 megabytes per second, meaning 1 PB would take over 210 days to transfer.
- HECC performance tweaks included:
 - Installed bbftp to allow Shift to eliminate ssh overhead.
 - Adjusted batch sizes and stream/thread counts to minimize Shift overhead and maximize individual system performance.
 - Provided Shift with information about additional ORNL resources to allow transfer parallelization.
- Once Shift was fully optimized, raw transfer performance increased to 1.08 gigabytes per second, reducing the time to transfer 1 PB to less than 11 days.

Mission Impact: By parallelizing transfers across multiple remote and local hosts in many-to-many fashion, HECC systems experts enabled the Shift transfer tool to take advantage of greater aggregate resources to maximize data transfer performance and reduce user turnaround time.

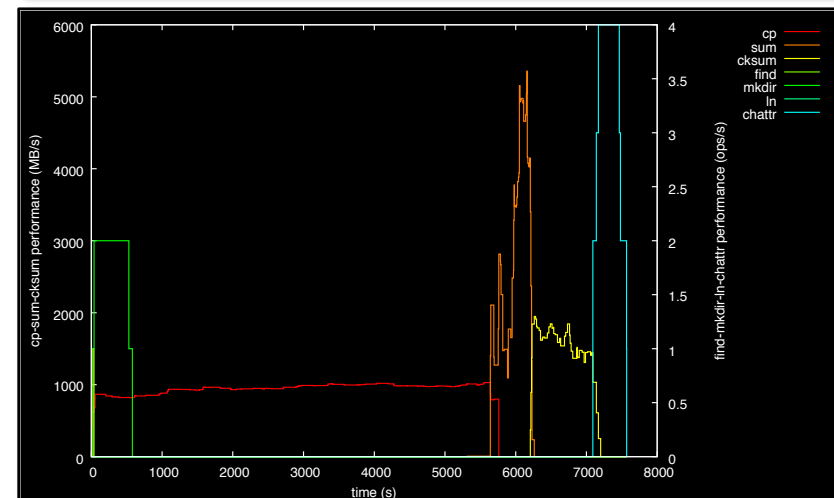


Chart showing the stages of a 6-terabyte transfer from Oak Ridge National Laboratory to the NAS facility, after optimization. Files are found on the file system, copied to the destination, checksummed at the source, verified at the destination, then file attributes are changed. Copy stage operated at around 1 gigabyte per second.

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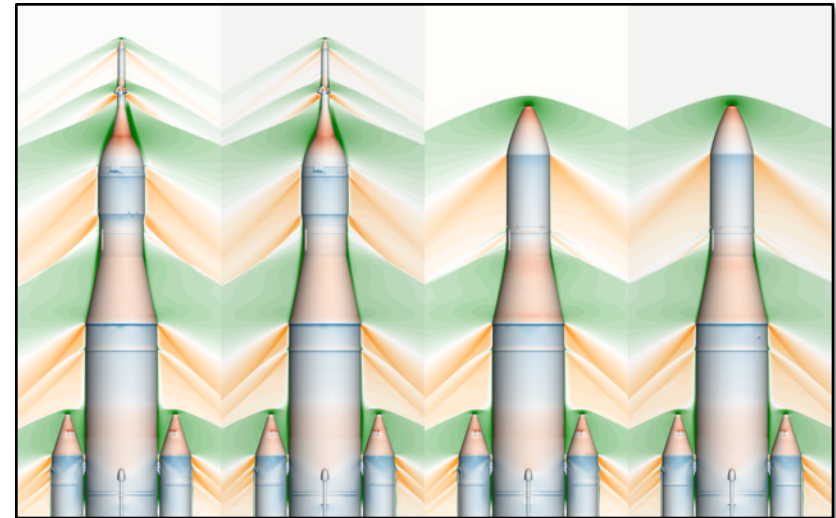
HECC Supercomputer Usage Sets New Record in March 2019



- In March, the combined usage of HECC supercomputers set a new record of 8,660,336 Standard Billing Units (SBUs).*
- The usage by 355 of NASA's science and engineering groups exceeded the previous record of 7,594,435 SBUs set in September 2018 by 1,065,901 SBUs.
- The record was achieved in great part by the Space Launch System using computational fluid dynamics (CFD) simulations focused on the prediction of the launch induced environment.
- Usage of Pleiades, Electra, Merope, and Endeavour contributed to this record.
- The top 10 projects used between 192,175 and 944,998 SBUs and together accounted for over 39% of the total usage.
- The HECC Project continues to evaluate and plan resources to address the future requirements of NASA's users.

* 1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.

Mission Impact: The increased capacity of HECC systems, along with working with users to optimize their run capacities, provides mission directorates with more resources to accomplish their goals and objectives.



SLS Block 1 cargo vehicle ascent and wind tunnel geometries showing flow fields. Left to right: EM-1 ascent; EM-1 wind tunnel; cargo ascent; cargo wind tunnel. Surfaces are colored by pressure contours, where blue is low and red is high. The green-white-orange colors represent low to high velocities. *Henry Lee, Stuart Rogers, NASA/Ames*

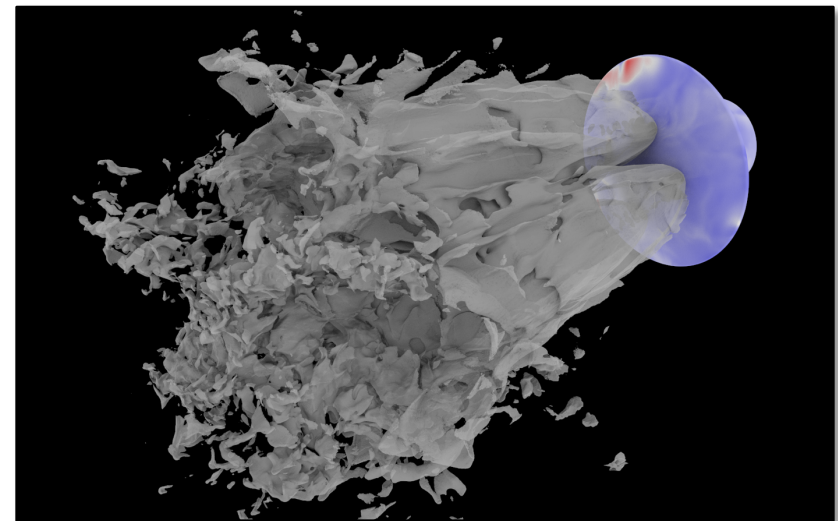
POC: Blaise Hartman, blaise.hartman@nasa.gov, (650)-604-2539,
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HECC Visualizations Featured in Talk on FUN3D Summit Runs at NVIDIA Conference



- User Eric Nielsen at NASA Langley presented “Unstructured Grid CFD Algorithms for NVIDIA GPUs” at the NVIDIA GPU Technology Conference (GTC) on March 20 in Silicon Valley.
 - He described preliminary results from runs on the Oak Ridge Leadership Computing Facility (OLCF) Summit supercomputer, supported by the OCLF INCITE program and Early Science grants.
 - Nielsen and Ashley Korzun, also at Langley, are co-principal investigators on the project.
- HECC provides ongoing visualization support for this research effort, including:
 - Developing custom code to work with the native domain decomposition used by FUN3D. Writing data in the native decomposition format enables much faster I/O for FUN3D, and can be done concurrently with the fluid dynamics calculations.
 - Delivering images and animations that help researchers gain insight into supersonic retropropulsion for large-vehicle Mars entry, such as the visualization results shown in Nielsen’s presentation.
- Among the technical challenges: computational runs are at high spatial and temporal resolution—1.14 billion vertices, 137 terabytes per run for large runs.

Mission Impact: HECC experts are collaborating with researchers at NASA Langley to study running the agency’s FUN3D application on a GPU-dominant architecture; specifically, the Summit system at the Oak Ridge Leadership Computing Facility—currently ranked first on the TOP500 list of the world’s most powerful supercomputers.



Snapshot from an animation showing the retropropulsion plumes of a Mars vehicle during the entry phase, with the vehicle surfaces colored by coefficient of pressure (low values in blue, high values in red).

Patrick Moran, NASA/Ames

POC: Patrick Moran, patrick.moran@nasa.gov, (650) 604-1660, NASA Advanced Supercomputing Division

HECC Deploys Upgrade to Lou Archive Storage System



- HECC engineers completed the upgrade of the Lou archive storage system after extensive testing. The refresh enhances the performance and capability of the system.
- The archive disk cache was expanded to nearly 8 petabytes (PB). This allows more data to reside on disk instead of being recalled from tape, and results in faster user access to data.
- With the faster disk subsystem and dedicated transfer nodes, the data transfer rate to and from the archive system has improved significantly. Multi-node transfers using six transfer nodes can attain up to a 100 percent performance improvement.
- The storage area network was converted from a Fiber Channel infrastructure to an InfiniBand infrastructure, which provides six times the bandwidth at lower cost.

Mission Impact: The HECC archive system upgrade provides NASA users with a highly available and scalable environment for long-term data storage.



The archive system servers, storage subsystems, and storage area network were refreshed as part of an upgrade in March 2019. As part of the archive system refresh, the Lou Data Analysis Nodes were refreshed, two with 1.5 terabytes of memory and two with 768 gigabytes of memory.

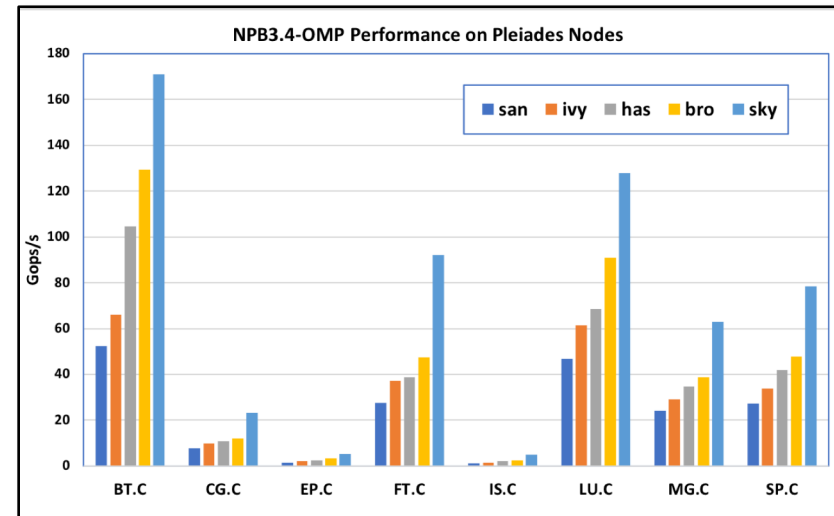
POC: Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NASA Advanced Supercomputing Division, ASRC

New Versions of the NAS Parallel Benchmarks Released



- HECC staff updated single- and multi-zone versions of the NAS Parallel Benchmarks (NPB). The new release (3.4) features:
 - A new class of problems (class F).
 - Use of modern programming language constructs to improve memory management and simplify the build process for the Message Passing Interface implementation.
 - Use of new language constructs to improve scalability of the OpenMP implementation.
- The NPBs mimic the computation and data movement in real-world CFD codes. The suite is widely used for:
 - Benchmarking and testing new systems.
 - Computer system procurement decisions.
 - Support in computer science research, such as programming languages and tools.
- Future work includes implementation of the NPBs for graphics processing units.
- For more information, see:
www.nas.nasa.gov/publications/npb.html

Mission Impact: NAS Parallel Benchmarks are used for performance evaluation in the procurement process of new supercomputer systems. Benchmark updates are important for system testing and for measuring capabilities of new computing technologies.



Node performance (Giga-operations per second) of the selected benchmarks from the NPB3.4 OpenMP version on Pleiades nodes. The chart illustrates performance improvement of different generations of the Intel Xeon processors that are deployed on Pleiades.

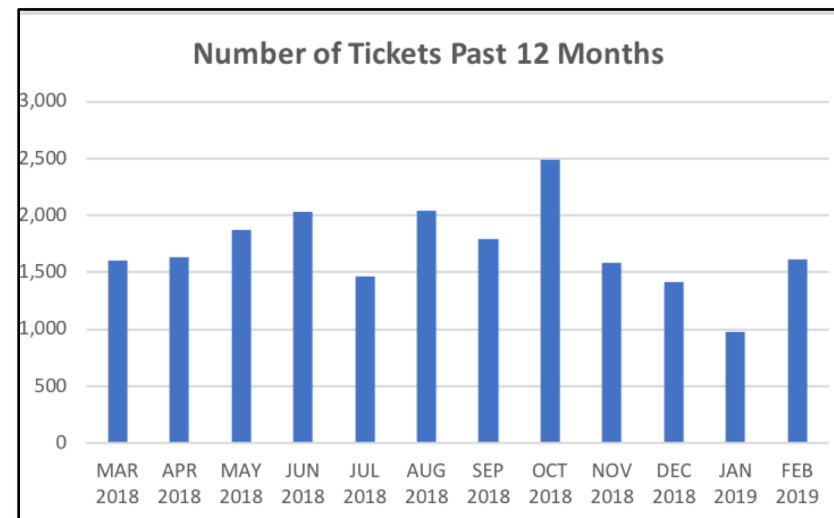
POC: Henry Jin, haoqiang.jin@nasa.gov, (650) 604-0165, NASA Advanced Supercomputing Division

HECC Staff Provide Outstanding, Continuous Support to Users



- During the past year, HECC staff provided support to more than 1,500 users from all mission directorates.
- Support staff across the HECC Project processed, tracked, and resolved just over 20,000 tickets for the 12 months from March 1, 2018 through February 28, 2019.
- Staff resolved tickets covering a wide range of activities originating from automated notification of system issues as well as user calls for help, including:
 - Restored connectivity to Pleiades and Electra.
 - Proactively detected when jobs didn't run, then contacted users to assist with job modifications within minutes of the original job's submission.
 - Continually modified allocations and account expiration dates.
 - Completed the New Operational Period (NOP) and helped to on-board remote users.
 - Closely communicated with users regarding systems outages and dedicated time.

Mission Impact: HECC's 24x7 support services staff resolve thousands of user and systems problems that enable users to focus on their mission projects vs. computer issues.



HECC staff resolved 20,502 tickets over the past 12 months, from March 1, 2018 through February 28, 2019. Peak numbers in October reflect support for users during the annual New Operational Period (NOP).

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HECC Networks Accomplishments: Change is in the Air



- The HECC Networks team has been working on some very exciting projects this year. Major projects include:
 - **EBPro/TIC:** Working to redesign the NAS high-speed network (NASLAN) to adhere to agency directives while maintaining the high performance required in a supercomputing environment.
 - **Wind Tunnels:** Collaborating with the Ames Wind Tunnel Systems Branch to implement a network that will enable near real-time analysis of wind tunnel data.
 - **NREN Transition:** Worked with Code I to transition the NASA Research and Engineering Network (NREN) to NAS, resulting in more cost-efficient, robust, high-speed interconnects to outside entities.
 - **Cloud:** Worked with HECC Systems staff to evaluate high-speed connectivity between NAS and Amazon Web Services.
 - **NASLAN Redesign:** Received approval of enhancements to NASLAN to provide improved high-availability between the core routers.
- The Networks team strives for high availability, secure resources, and maximum performance for our scientific community.

Mission Impact: Continually improving the HECC networking environment at the NASA Advanced Supercomputing facility enables scientists to move vast amounts of data securely and at maximum performance, reducing time-to-solution for important agency projects.



HECC networking experts support users across the U.S. and around the world. The team works closely with users to optimize their end-to-end flows, and collaborates with other network teams to improve throughput.

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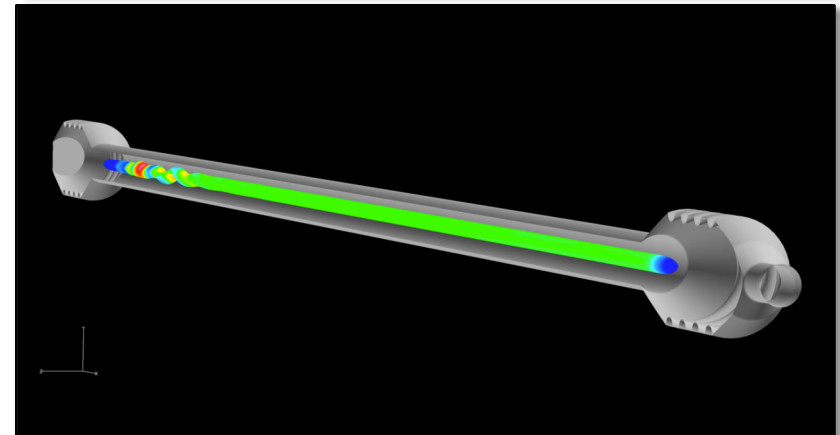
Extreme Plasma Modeling for Planetary Entry and Space Exploration*



- Researchers are running magnetohydrodynamics (MHD) simulations of the NASA Ames Arc Jet Complex's Aerodynamic Heating Facility on Pleiades to better understand the complex plasma flow behavior inside arc jet wind tunnels.
 - Arc jets produce highly energetic plasma flows to replicate extreme aerothermal heating experienced by spacecraft during planetary entry, in order to evaluate the performance of thermal protection system materials.
 - The Pleiades simulations, run using the NASA-developed ARC Heater Simulator (ARChES) analysis tool, provide insight into the radiative transfer, magnetic field, imposed electric current density, and turbulence present in arc jet heaters.
- Findings include:
 - Strong gradients in both the fluid and electromagnetic fields give rise to upstream kink instabilities that drive the arc attachment at the electrodes.
 - The magnetic field plays an essential role in characterizing the flow between the anode chamber and the nozzle throat.
- These findings aid validation & verification against experimental results, and can also inform maintenance schedules and facility upgrades.

* HECC provided supercomputing resources and services in support of this work.

Mission Impact: The ARChES simulations help engineers better understand the operational envelope of the NASA Ames Arc Jet Complex, a facility that is critical to the evaluation of thermal protection system materials. The tool's capabilities may also be extended to other technologies, such as in-space propulsion.



This video shows the result of a two-week long simulation—representing a half-second in real-time—of the Aerodynamic Heating Facility at NASA Ames, using 1,200 processors on the Pleiades supercomputer. The isosurface represents the electric current density. High magnitudes of the total magnetic field are shown in red, lower range is shown in blue. *Jeremie B.E. Meurisse, Nagi N. Mansour, NASA/Ames*

POCs: Sander Visser, sander.j.visser@nasa.gov, (650) 604-5248, NASA Advanced Supercomputing (NAS) Division, University of Illinois at Urbana-Champaign;
Nagi Mansour, nagi.n.mansour@nasa.gov, (650) 604-6420, NAS Division

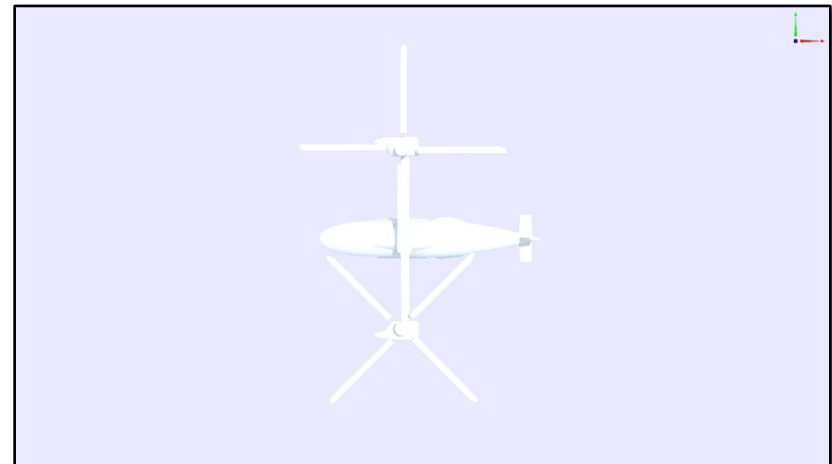
Towards Urban Air Mobility: Side-By-Side Air Taxi Simulations*



- Aerodynamics engineers at NASA Ames produced high-fidelity computational fluid dynamics (CFD) simulations of a side-by-side rotor air taxi concept to accurately predict vehicle performance. Results show:
 - The side-by-side air taxi has intermeshing rotors. The overlapping rotors in cruise flight are more efficient than two non-overlapping rotors, and have a more compact configuration.
 - The interactions between multiple rotors and the fuselage emerged as an important factor to consider in the design of safer, more efficient, and quieter vehicles.
- The fluid equations were solved on grids comprising hundreds of millions of grid points, using the Pleiades and Electra supercomputers.
- Results from the simulations can also be used to calibrate and validate low-fidelity design tools.

* HECC provided supercomputing resources and services in support of this work.

Mission Impact: HECC's powerful supercomputing resources enable complex fluid equations to predict rotorcraft performance for Urban Air Mobility vehicles to be solved in just a few days, instead of months.



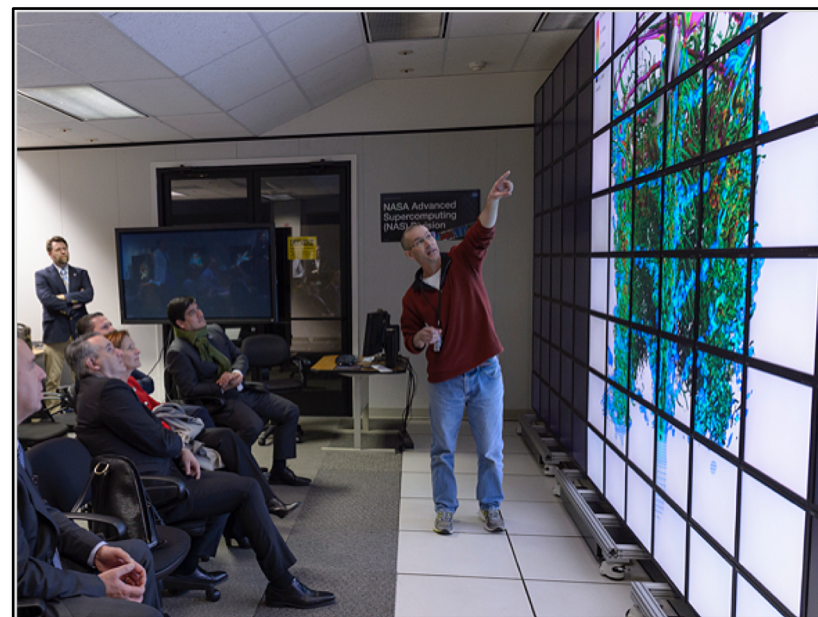
Visualization of the flow of NASA's side-by-side concept rotorcraft for urban air mobility (UAM) in forward flight. The vortex wake reveals the complex interactions between the intermeshing rotors. Vortices are colored by vorticity magnitude, where red is high vorticity and blue is low vorticity. Below and behind the rotorcraft, pressure waves show the acoustic field.
Patricia Ventura Diaz, NASA/Ames

POCs: Patricia Ventura Diaz, patricia.venturadiaz@nasa.gov, (650) 604-0075, NASA Advanced Supercomputing (NAS) Division, Science and Technology Corp.;
Seokkwan Yoon, s.yoon@nasa.gov, (650) 604-4482, NAS Division

HECC Facility Hosts Several Visitors and Tours in March 2019



- HECC hosted 14 tour groups in March; these guests learned about the agency-wide missions being supported by HECC assets, and also viewed the D-Wave 2000Q quantum computer system. Visitors this month included:
 - His Excellency Carlos Alvarado Quesada, President of the Republic of Costa Rica; H.E. Dyalá Jiménez Figueres, Minister of Foreign Trade; H.E. Luis Adrián Salazar, Minister of Science, Technology and Telecommunications; and H.E. Fernando Llorca, Costa Rica's Ambassador to the U.S.
 - An agency group including: Pam Millar, Director, NASA Earth Science Technology Office; Mike Little, Program Manager, Advanced Information Systems Technology; Jacqueline LeMoigne, Deputy for New Observing System Strategy; and Marge Cole, Deputy, Advanced Information Systems Technology.
 - A group of participants from the Defense Advanced Research Project Agency's Service Chiefs Fellowship Program.
 - Several education groups also visited the NAS facility during this period.



NASA Advanced Supercomputing (NAS) Division Visualization Group Lead Chris Henze presents to a delegation from the Republic of Costa Rica. President Alvarado Quesada is seated front row, far right.

POC: Gina Morello, gina.f.morello@nasa.gov, (650) 604-4462,
NASA Advanced Supercomputing Division



- **“EagerMap: A Task Mapping Algorithm to Improve Communication and Load Balancing in Clusters of Multicore Systems,”** E. Cruz, M. Diener, L. Pilla, P. Navaux, ACM Transactions on Parallel Computing, vol. 5, issue 4, March 2019. *
<https://dl.acm.org/citation.cfm?doid=3314574.3309711>
- **“Cosmic Ray Acceleration of Cool Clouds in the Circumgalactic Medium,”** J. Wiener, E. Zweibel, M. Ruszkowski, arXiv:1903.01471 [astro-ph.GA], March 4, 2019. *
<https://arxiv.org/abs/1903.01471>
- **“Is It Possible to Reconcile Extragalactic IMF Variations with a Universal Milky Way IMF?”** D. Guszejnov, P. Hopkins, A. Graus, Monthly Notices of the Royal Astronomical Society, March 13, 2019. *
<https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/stz736/5379463>
- **“A Hot Rocky and Warm Puffy Super-Earth Orbiting TOI-420 (HD 15337),”** X. Dumusque, et al., arXiv:1903.05419 [astro-ph.EP], March 13, 2019. *
<https://arxiv.org/abs/1903.05419>
- **“A Super-Earth and Two Sub-Neptunes Transiting the Bright, Nearby, and Quiet M-Dwarf TOI-270,”** M. Günther, et al., arXiv:1903.06107 [astro-ph.EP], March 14, 2019. *
<https://arxiv.org/abs/1903.06107>
- **“Toward Noise Certification During Design: Airframe Noise Simulations for Full-Scale, Complete Aircraft,”** M. Khorrami, E. Fares, CEAS Aeronautical Journal, March 16, 2019. *
<https://link.springer.com/article/10.1007/s13272-019-00378-1>

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)



- **“HD 213885b: A Transiting 1-Day-Period Super-Earth with an Earth-Like Composition Around a Bright ($V = 7.9$) Star Unveiled by TESS,”** N. Espinoza, et al., arXiv:1903.07694 [astro-ph.EP], March 18, 2019. *
<https://arxiv.org/abs/1903.07694>
- **“Dancing in the Dark: Uncertainty in Ultrafaint Dwarf Galaxy Predictions from Cosmological Simulations,”** F. Munshi, et al., The Astrophysical Journal, vol. 874, no. 1, March 19, 2019. *
<https://iopscience.iop.org/article/10.3847/1538-4357/ab0085/meta>
- **“Studying the Physical Properties of Tidal Features I. Extracting Morphological Substructure in CANDELS Observations and VELA Simulations,”** K. Mantha, et al., Monthly Notices of the Royal Astronomical Society (accepted), March 27, 2019. *
<https://academic.oup.com/mnras/advance-article-abstract/doi/10.1093/mnras/stz872/5420844>
- **“Nonlinear Evolution of Ion Kinetic Instabilities in the Solar Wind,”** L. Ofman, arXiv:1903.11343 [physics.space-ph], March 27, 2019. *
<https://arxiv.org/abs/1903.11343>
- **“Sensitivity to Physical and Numerical Aspects of Large-Eddy Simulation of Stratocumulus,”** G. Matheou, J. Teixeira, Monthly Weather Review (accepted), March 29, 2019. *
<https://journals.ametsoc.org/doi/abs/10.1175/MWR-D-18-0294.1>
- **“A Regularized Deconvolution Method for Turbulent Closure Modeling in Implicitly Filtered Large-Eddy Simulation,”** Q. Wang, M. Ihme, Combustion and Flame, vol. 204 (June), available online March 29, 2019. *
<https://www.sciencedirect.com/science/article/pii/S0010218019301038>

* HECC provided supercomputing resources and services in support of this work



- **NASA's Pleiades Simulates Launch Abort Scenarios**, *HPCwire*, March 15, 2019—Cutting-edge simulations run on the Pleiades supercomputer help engineers shape the final configuration of the Orion launch abort vehicle, designed to keep astronauts safe during launch.
<https://www.hpcwire.com/2019/03/15/nasas-pleiades-simulates-launch-abort-scenarios/>
 - Based on a NAS Feature Story from March 2018:
https://www.nas.nasa.gov/publications/articles/feature_Orion_acoustics_Cadieux.html
 - Original story was also reposted by HPCwire:
<https://www.hpcwire.com/off-the-wire/helping-keep-astronauts-safe-with-advanced-simulations-visualizations/>
- **Galactic Center Visualization Delivers Star Power**, *Chandra X-Ray Observatory Press Release*, March 22, 2019—By combining NASA Ames supercomputer simulations with data from NASA's Chandra X-ray Observatory, a new immersive, ultra-high-definition visualization provides a fresh perspective on what is happening in and around the center of the Milky Way.
<http://chandra.si.edu/photo/2019/gcenter/>

News and Events: Social Media



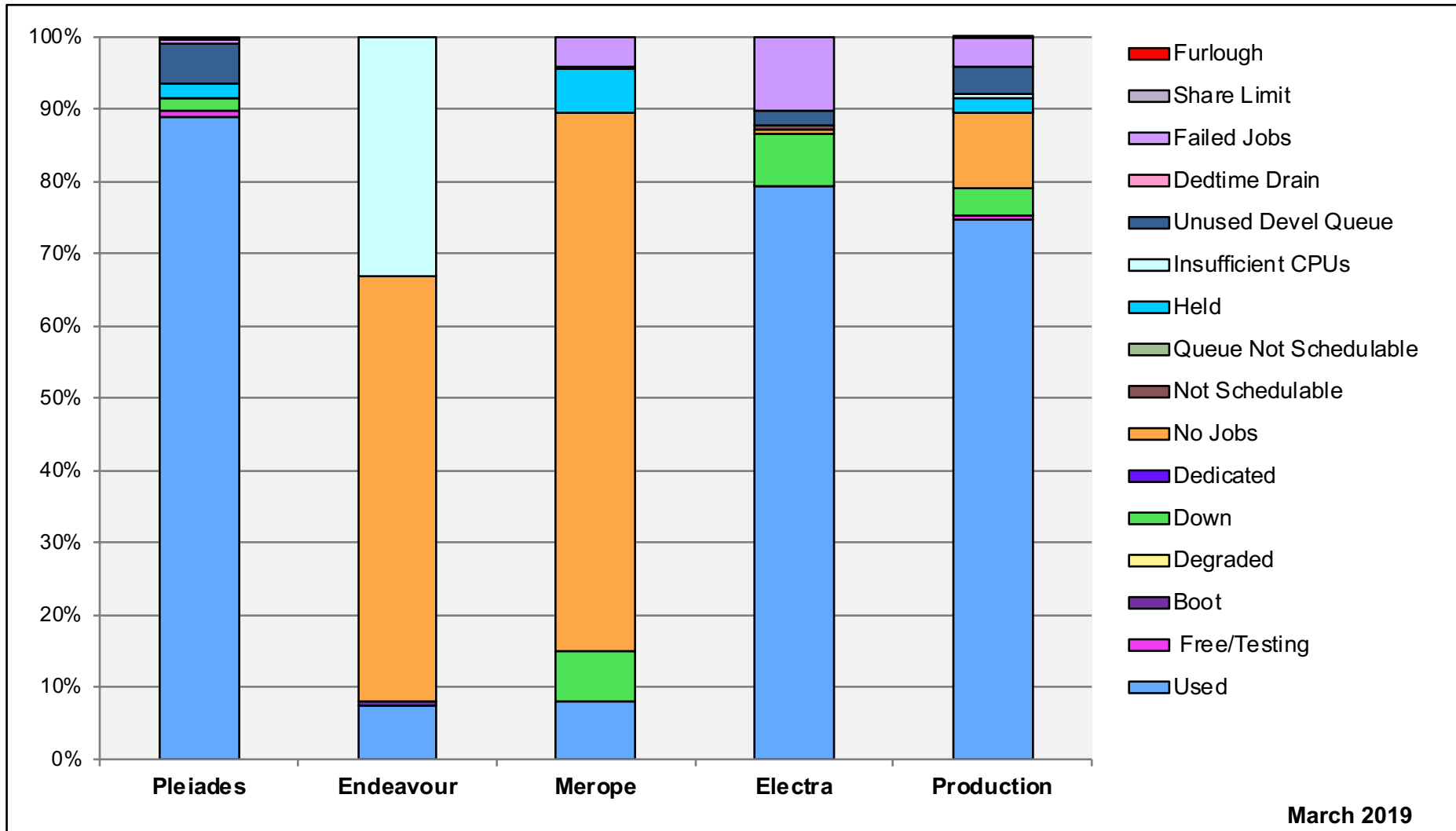
- **Agency Coverage of NAS Computing**

- NASA (HQ) coverage of Chandra X-Ray Observatory galaxy simulation:
 - [Facebook](#): 4.3k reactions, 434 shares (Image being used as their cover/banner as of March 23)
 - [Twitter](#): 1,376 retweets, 5,114 likes
- NASA Ames coverage of Chandra X-Ray Observatory galaxy simulation:
 - [Twitter](#): 89 retweets, 217 likes
 - [Facebook](#): 497 users reached, 44 engagements
- Chandra X-Ray Observatory coverage of galaxy simulation:
 - [Twitter](#): 106 retweets, 250 likes
 - [Facebook](#): 654 reactions, 178 shares
 - [YouTube](#): 268,735 views, 2.3k likes

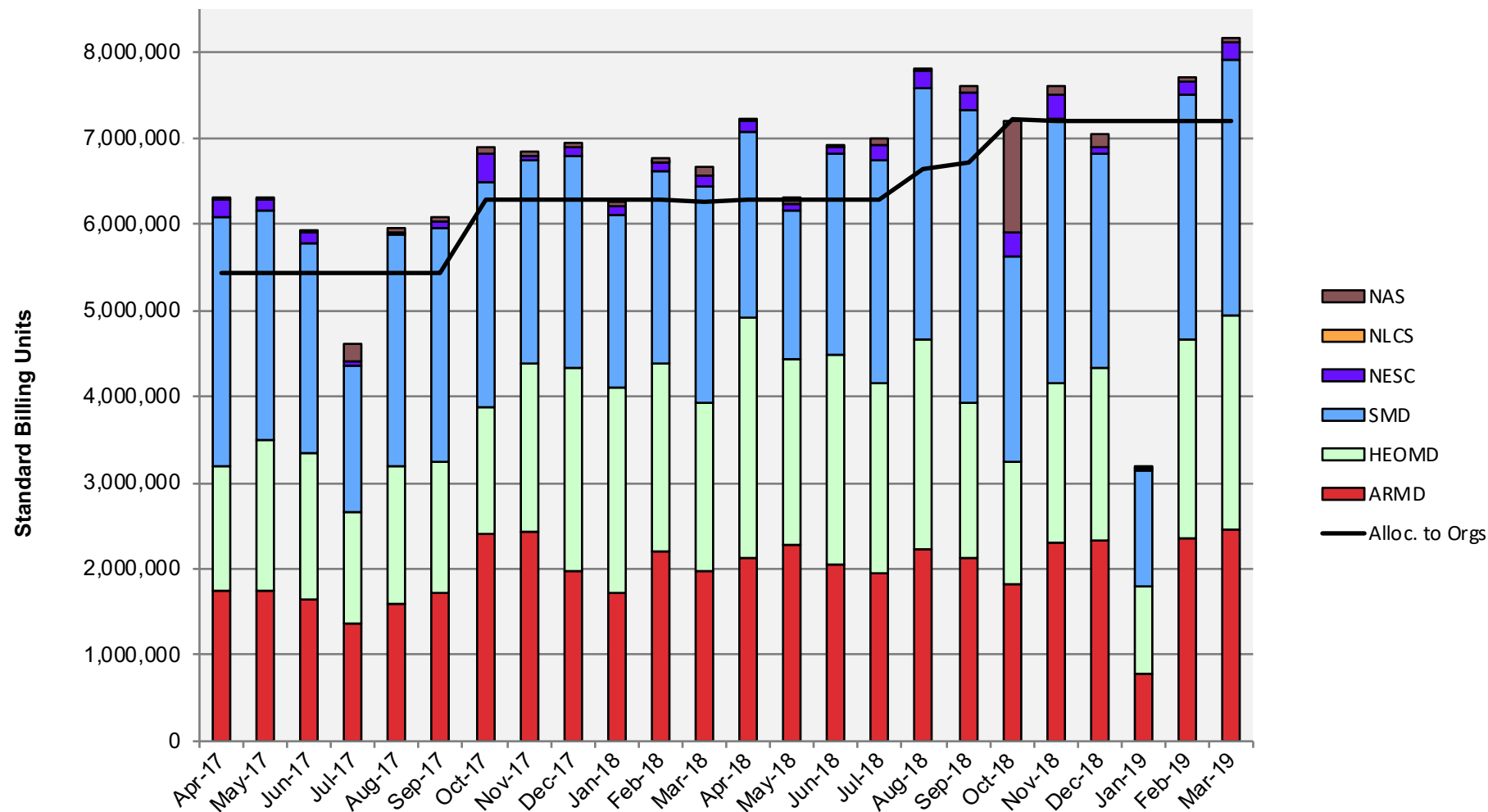
- **Top Posts from NAS**

- 32nd Anniversary of the NAS facility
 - [Twitter](#): 1 retweet, 17 likes
 - [Facebook](#): 639 users reached, 106 engagements
- Orion Launch Abort System simulations
 - [Twitter](#): 113 retweets, 366 likes
- Coverage of Chandra X-Ray Observatory galaxy simulation
 - [Twitter](#): 12 retweets, 41 likes
 - [Facebook](#): 194 users reached, 18 engagements
- Solar Eclipse Prediction simulation story
 - [Facebook](#): 125 users reached, 5 engagements

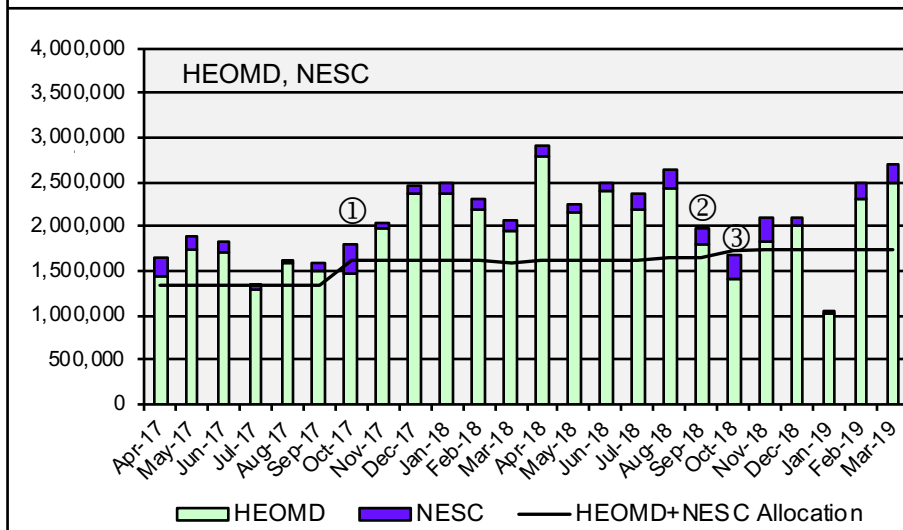
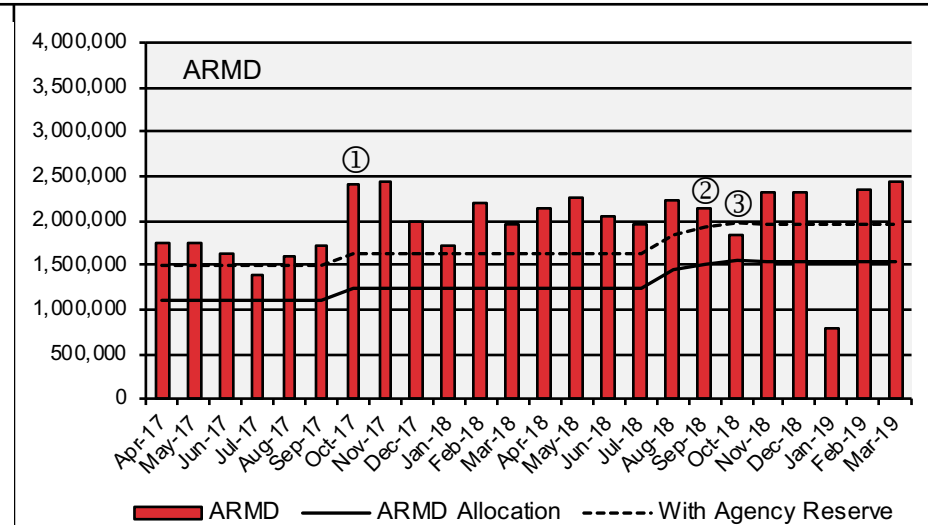
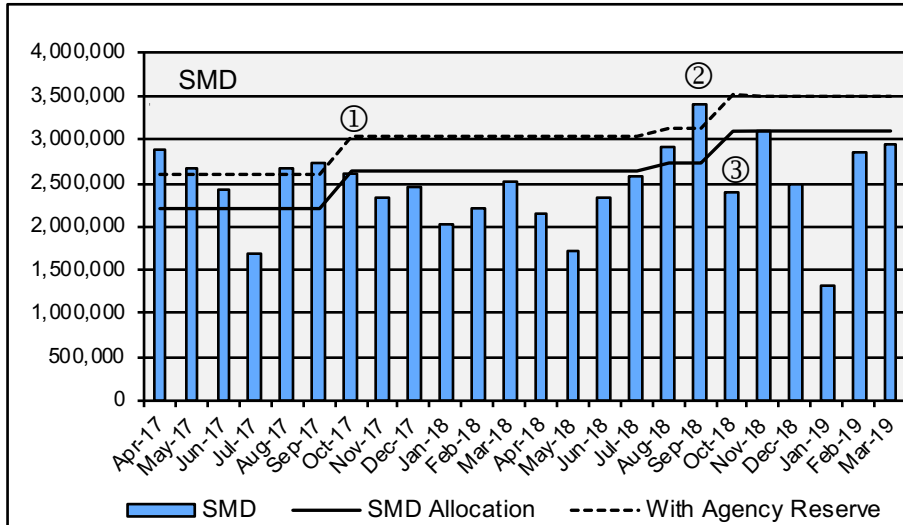
HECC Utilization



HECC Utilization Normalized to 30-Day Month

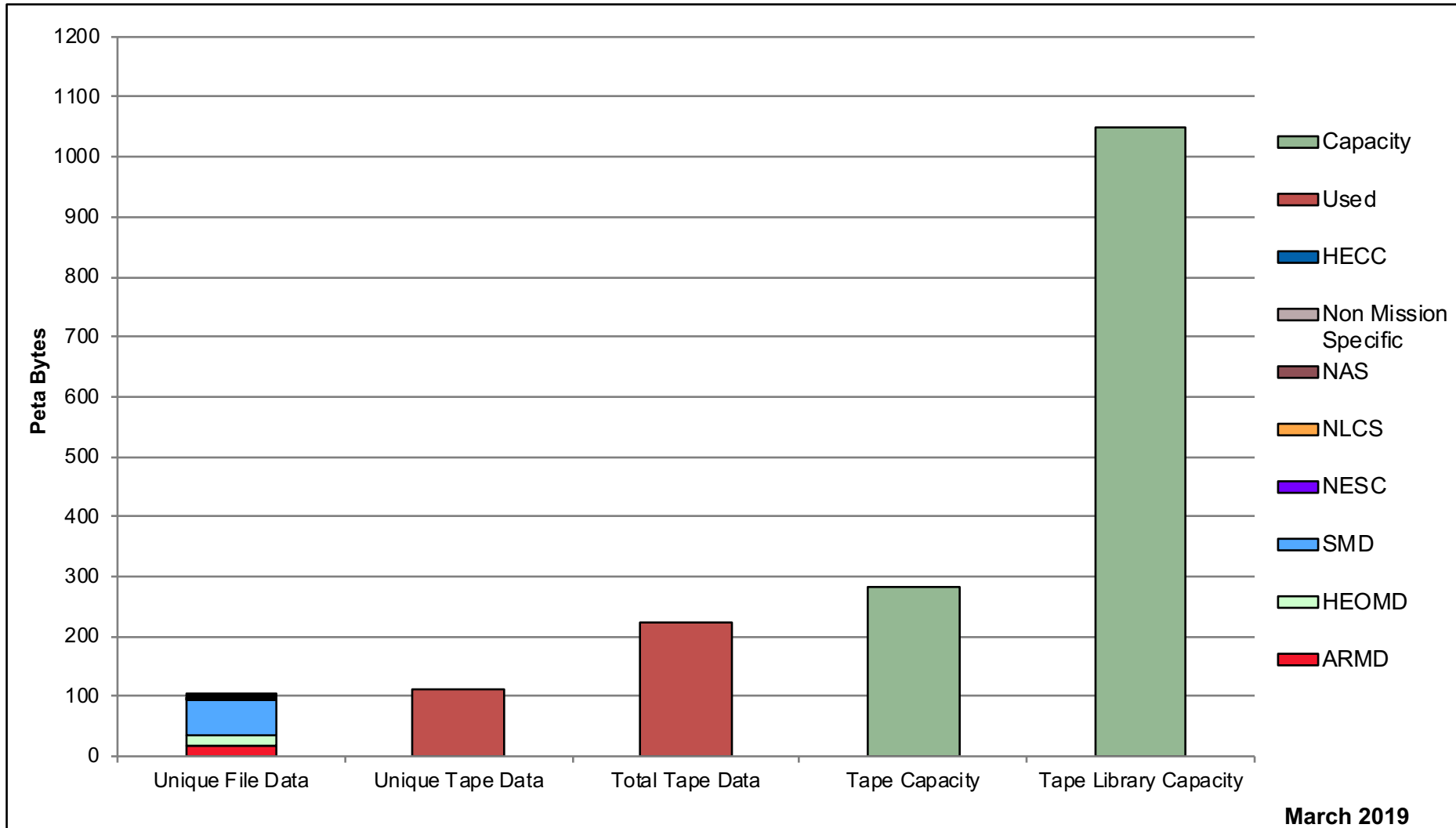


HECC Utilization Normalized to 30-Day Month



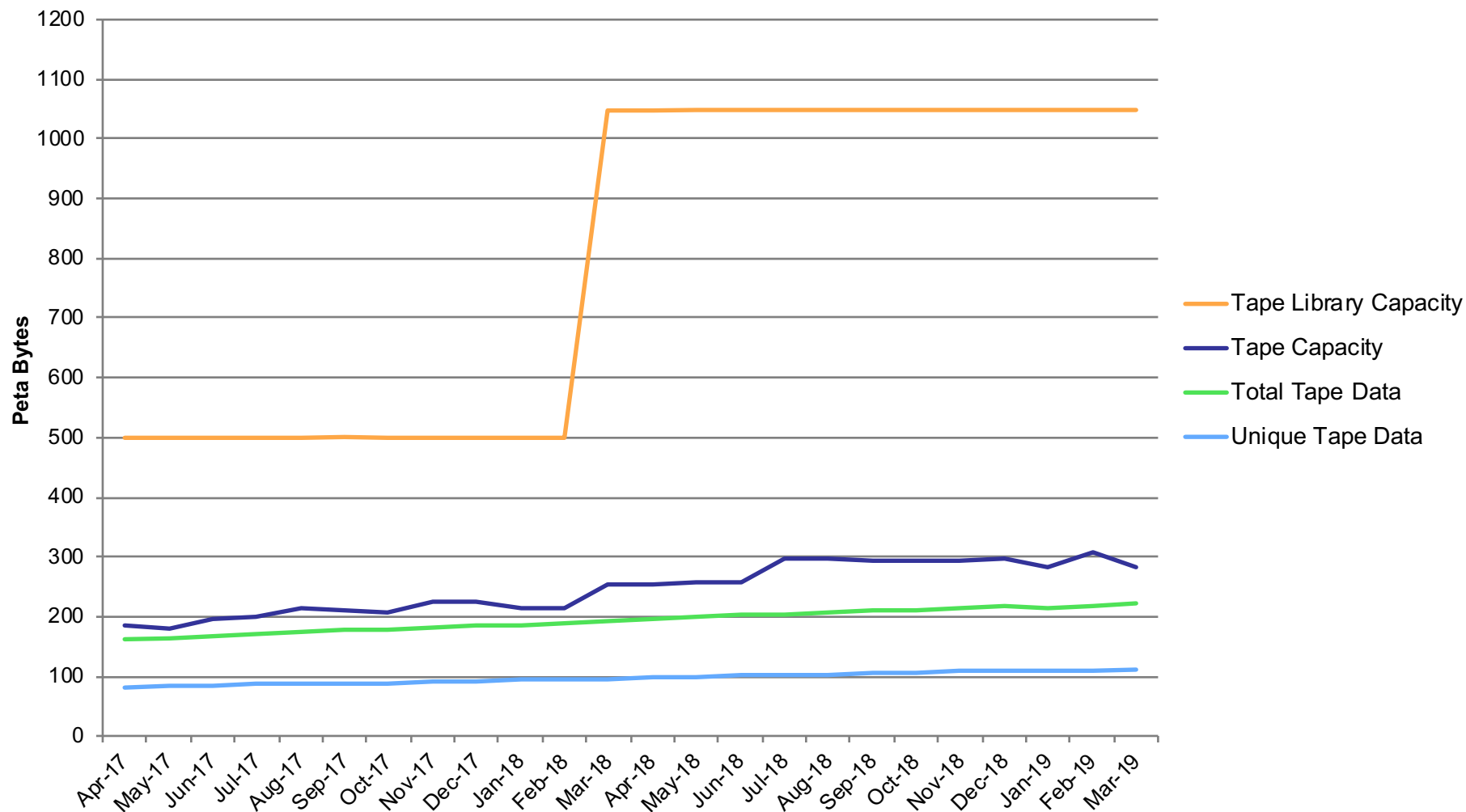
- ① 4 Skylake E cells (16 D Rack Equivalence) added to Electra
- ② 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to ARMD
- ③ 2 Skylake E cells (8 D Rack Equivalence) added to Electra; 1 rack is dedicated to SMD

Tape Archive Status

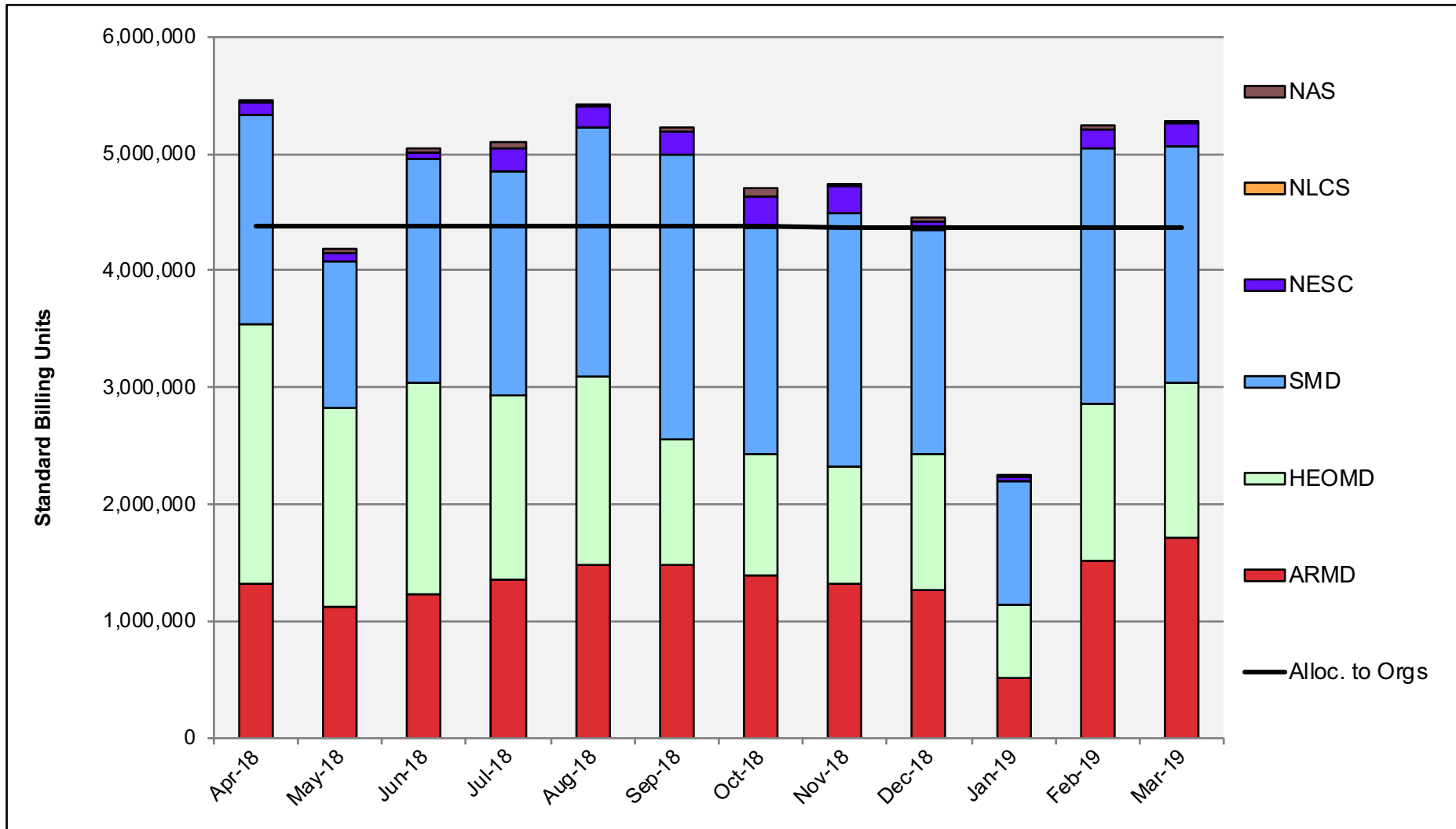


March 2019

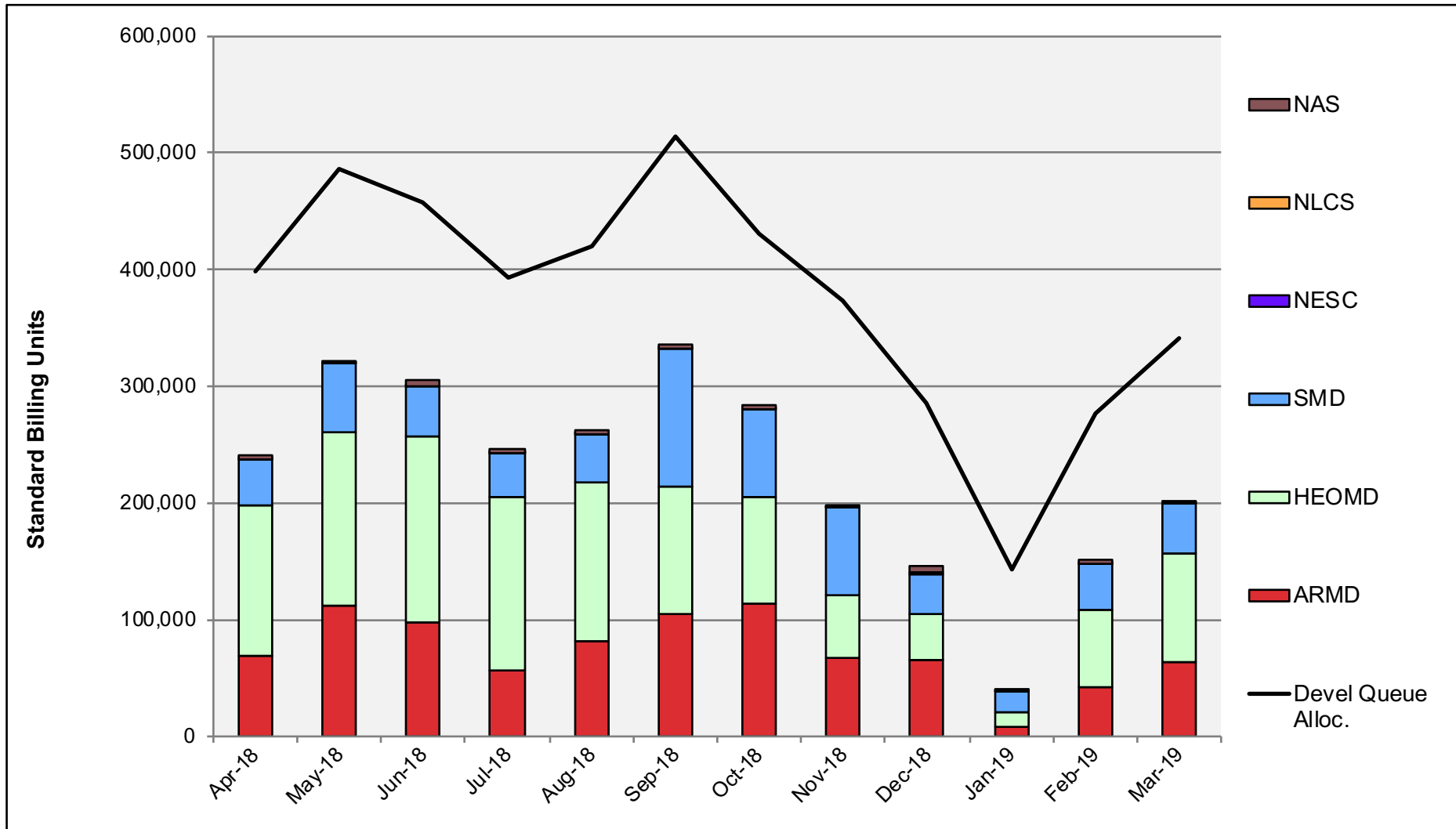
Tape Archive Status



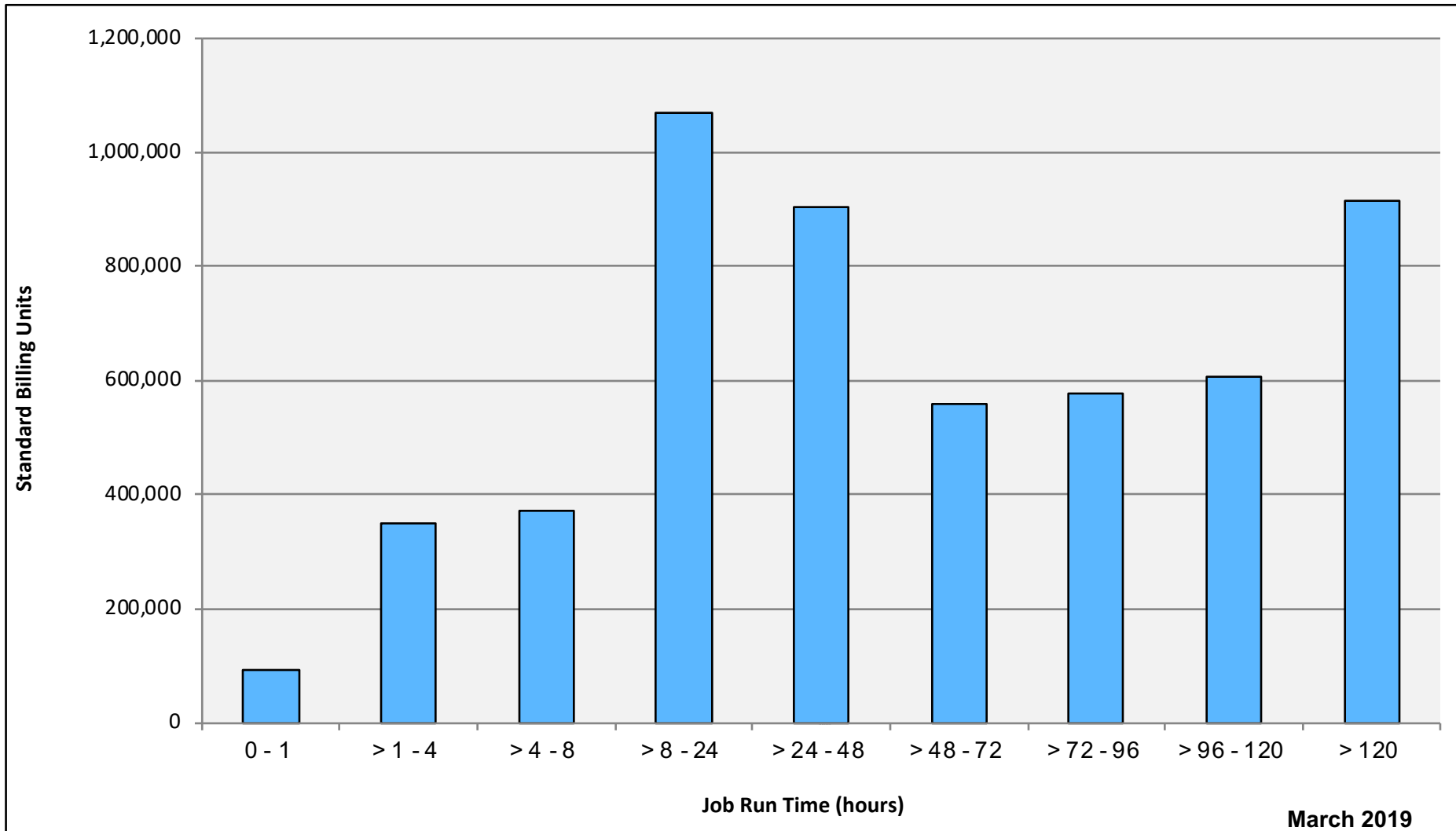
Pleiades: SBUs Reported, Normalized to 30-Day Month



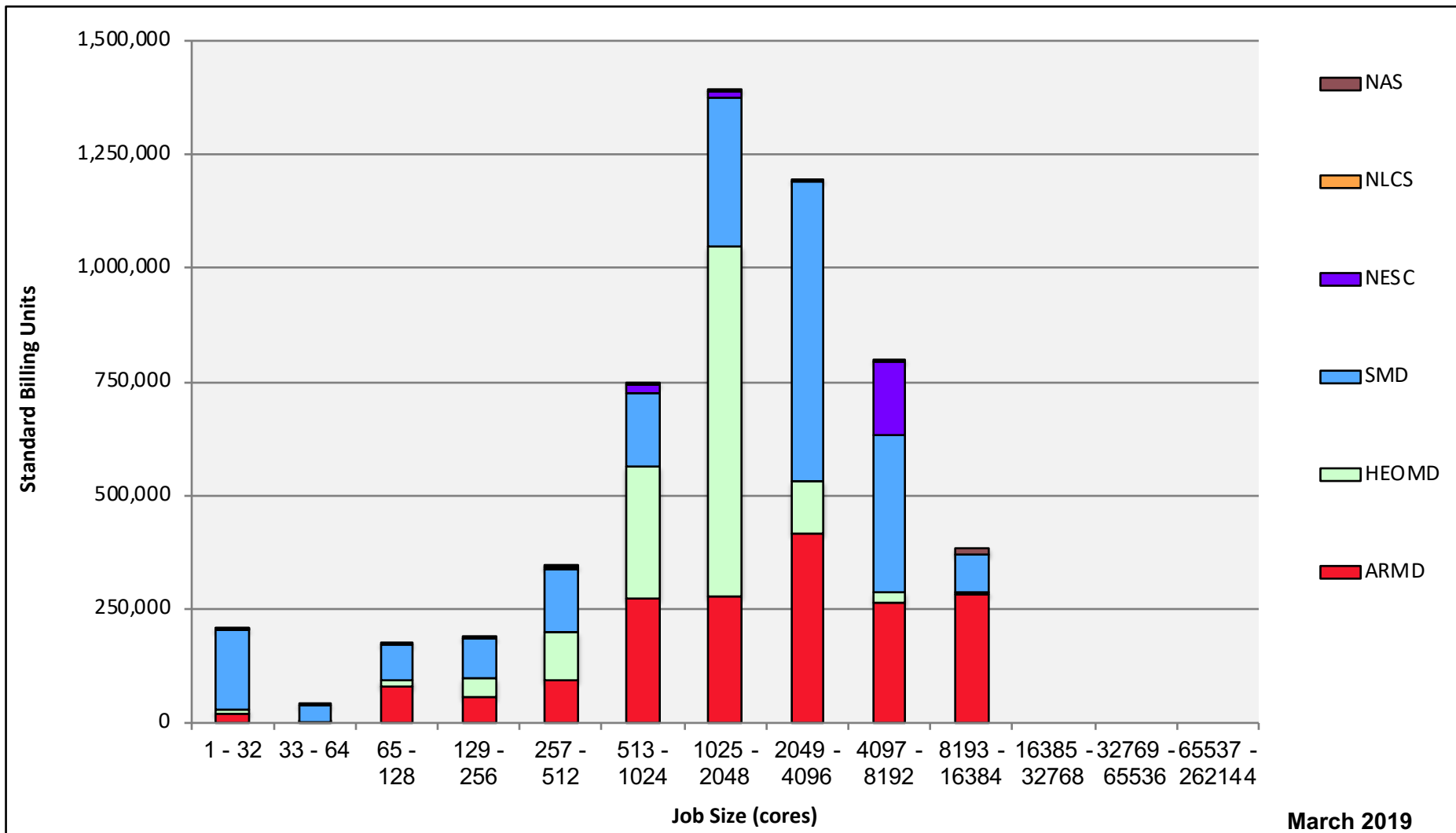
Pleiades: Devel Queue Utilization



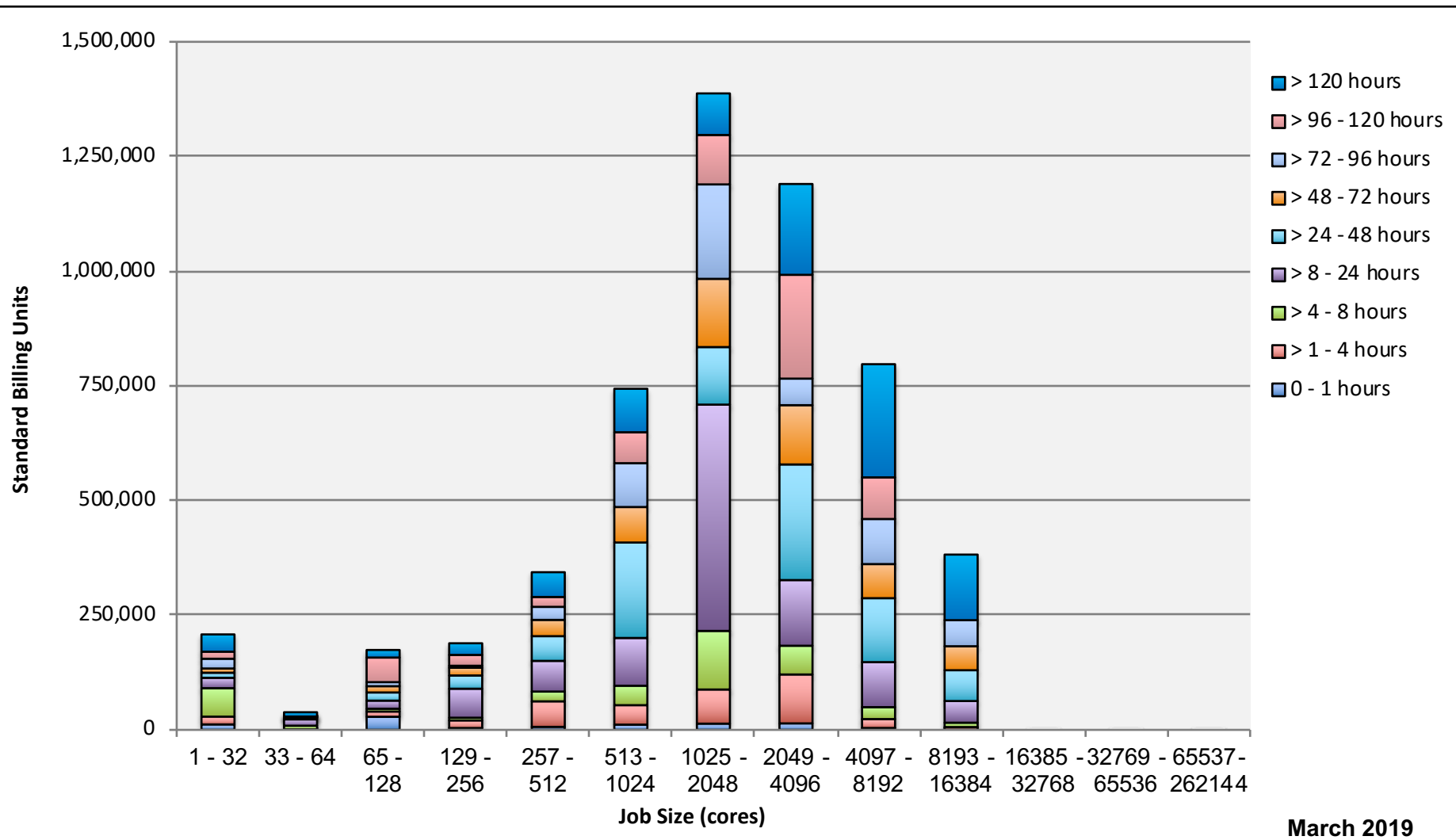
Pleiades: Monthly Utilization by Job Length



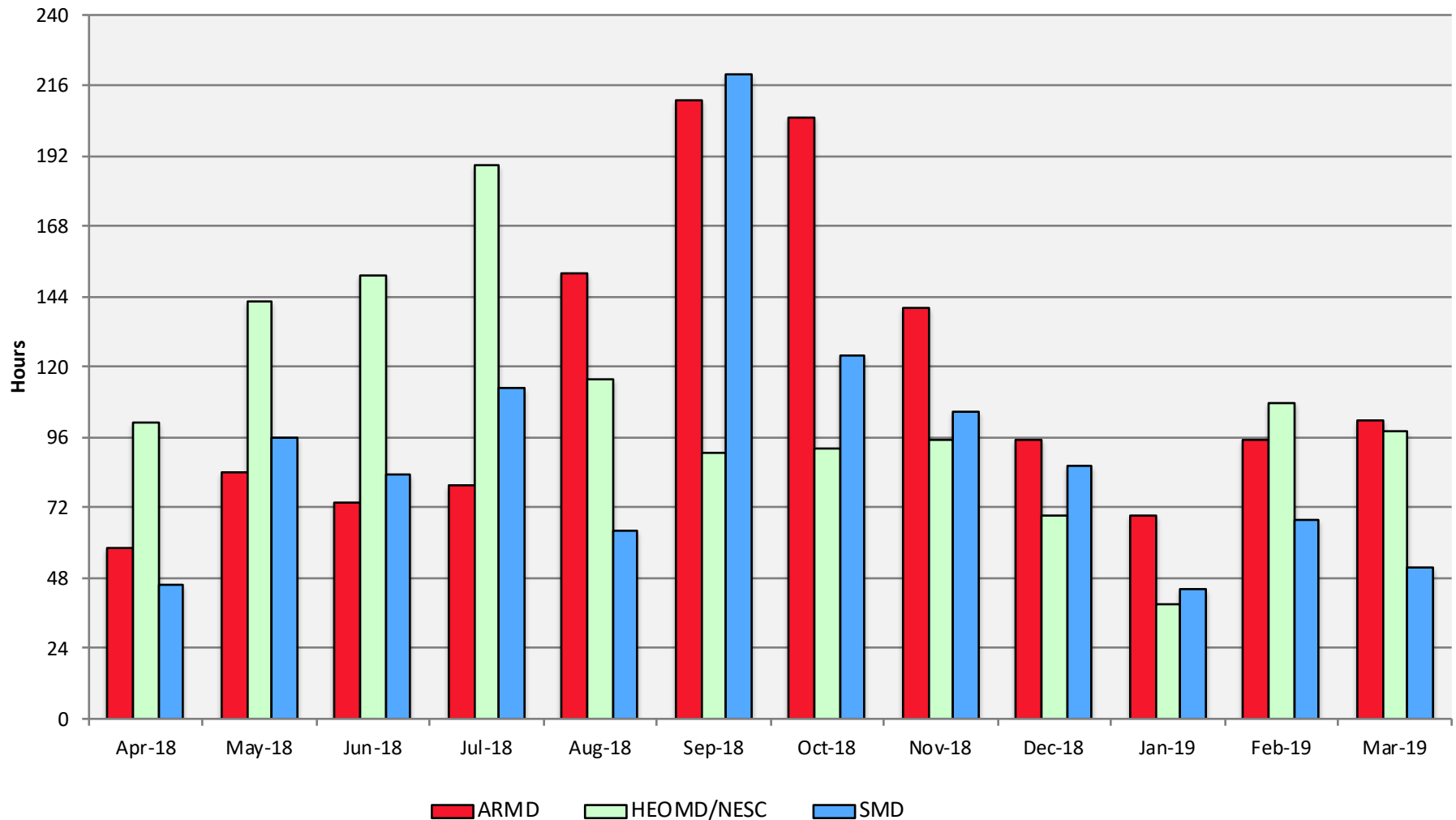
Pleiades: Monthly Utilization by Size and Mission



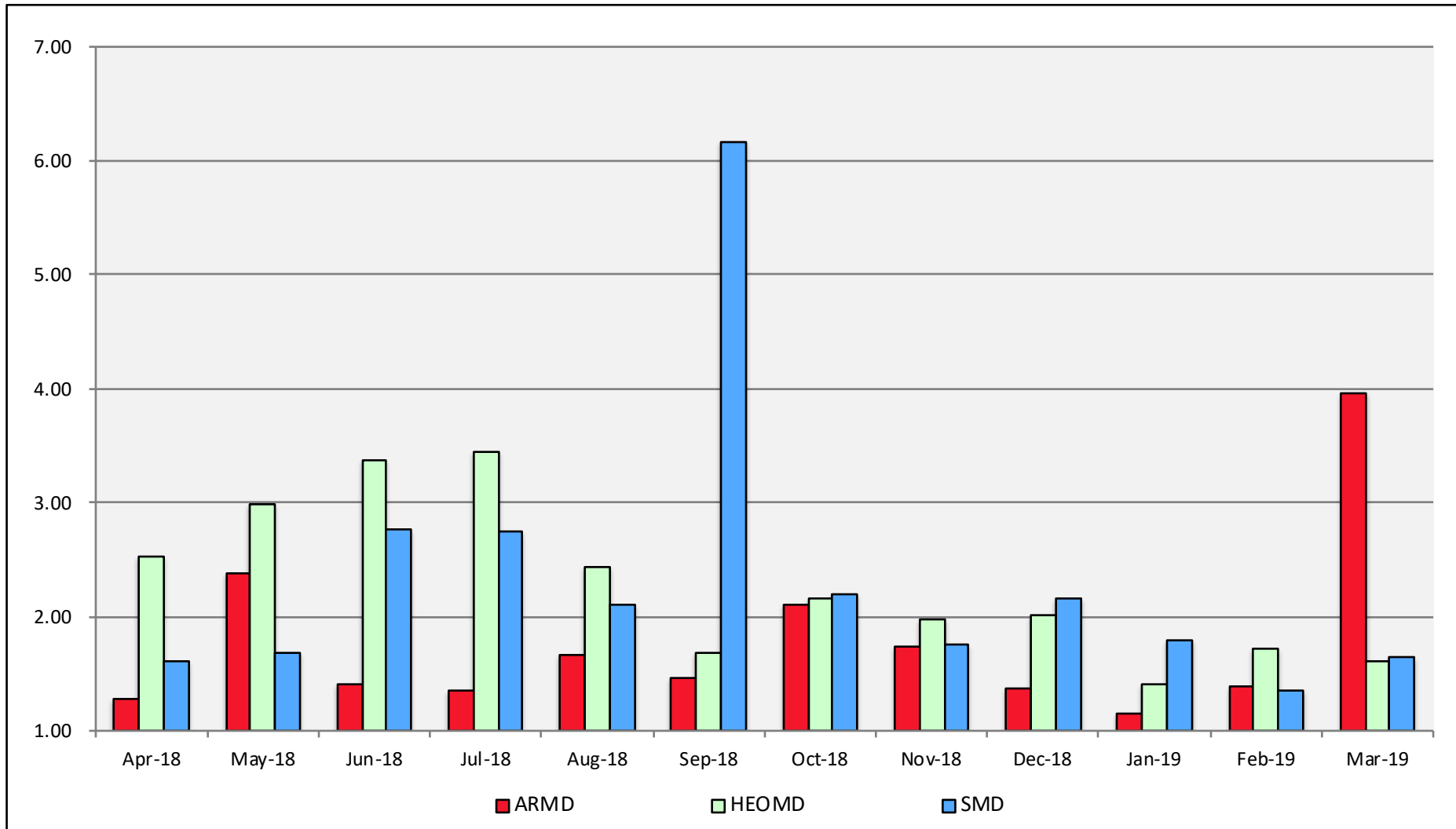
Pleiades: Monthly Utilization by Size and Length



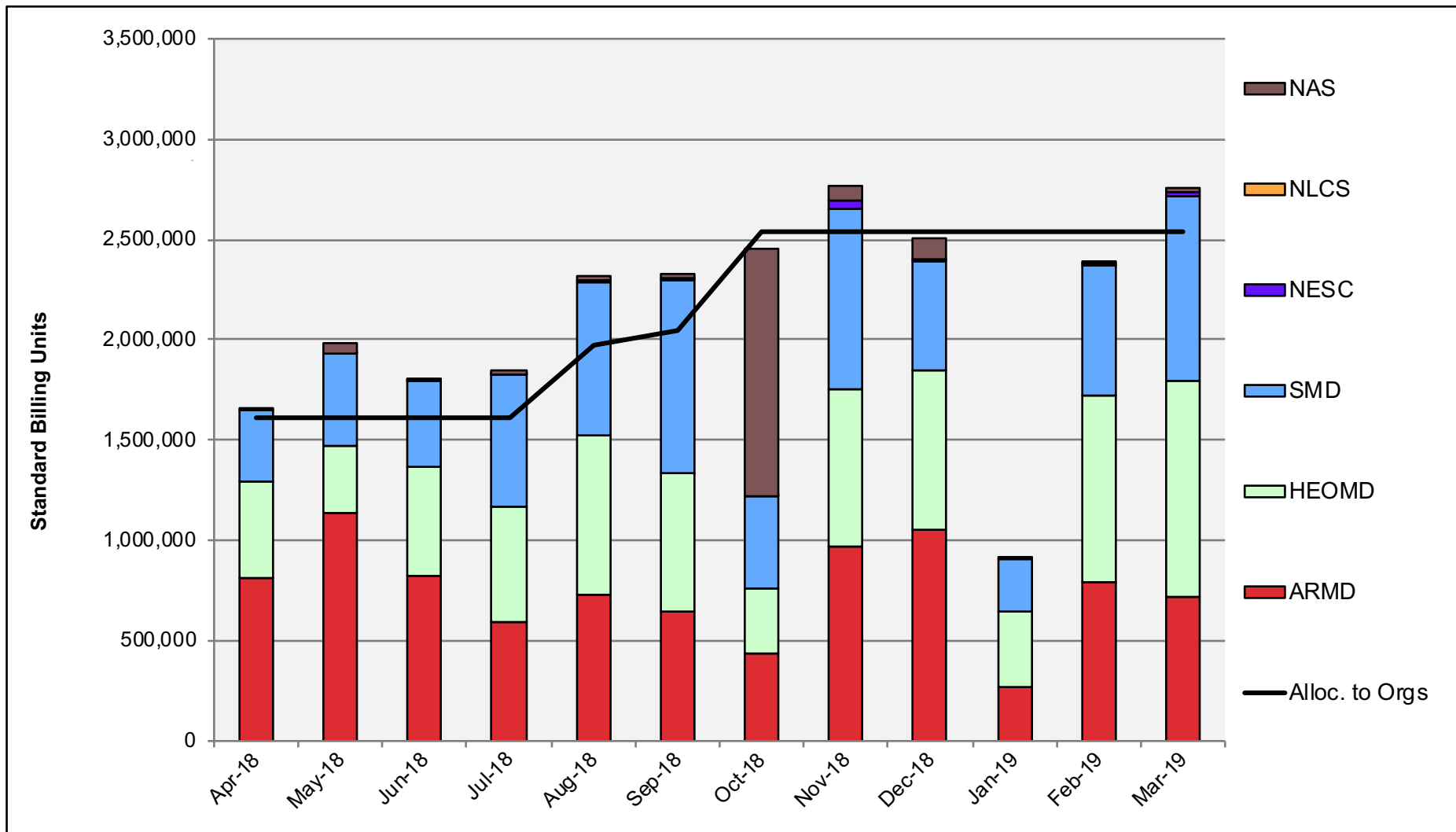
Pleiades: Average Time to Clear All Jobs



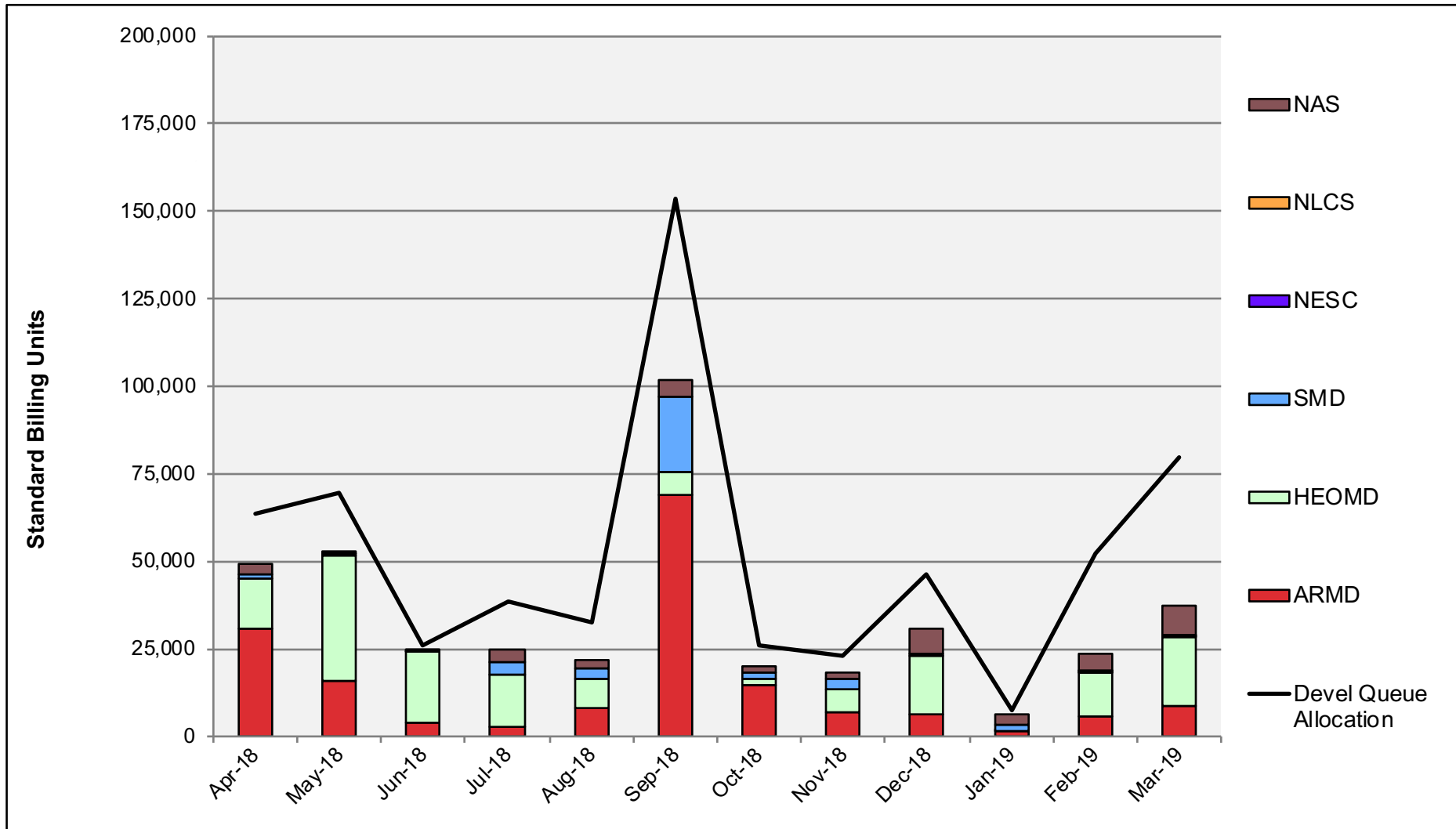
Pleiades: Average Expansion Factor



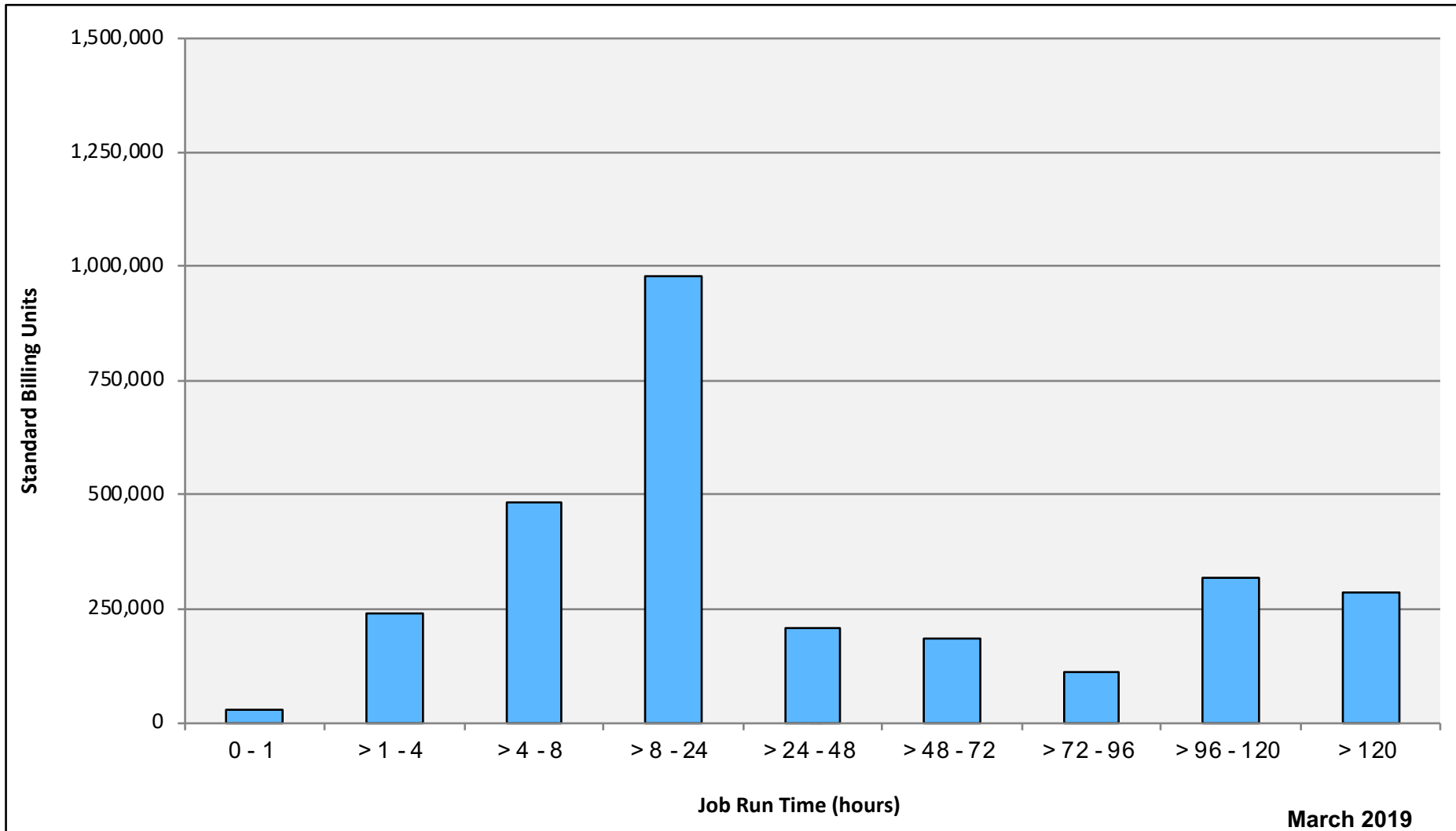
Electra: SBUs Reported, Normalized to 30-Day Month



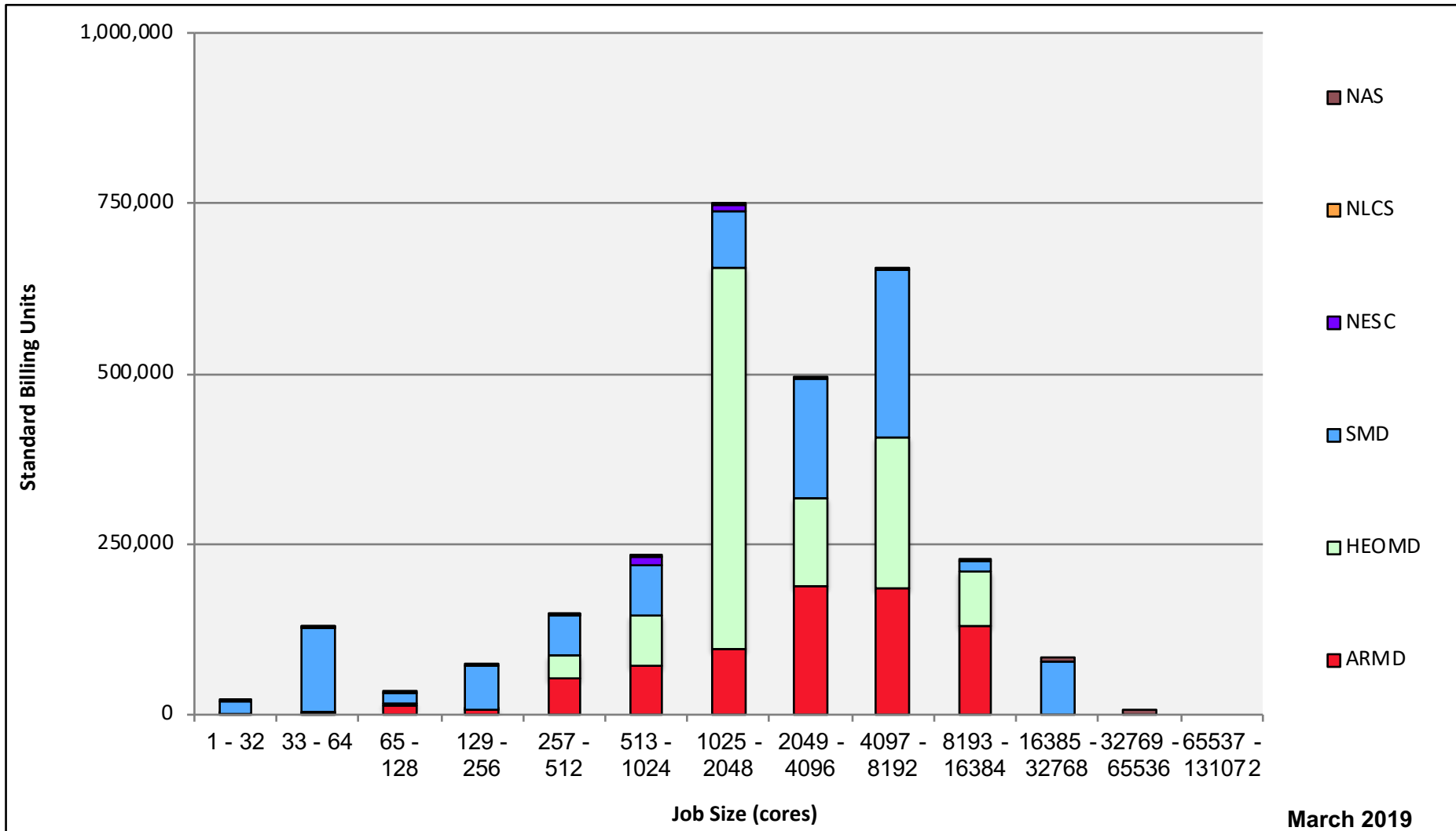
Electra: Devel Queue Utilization



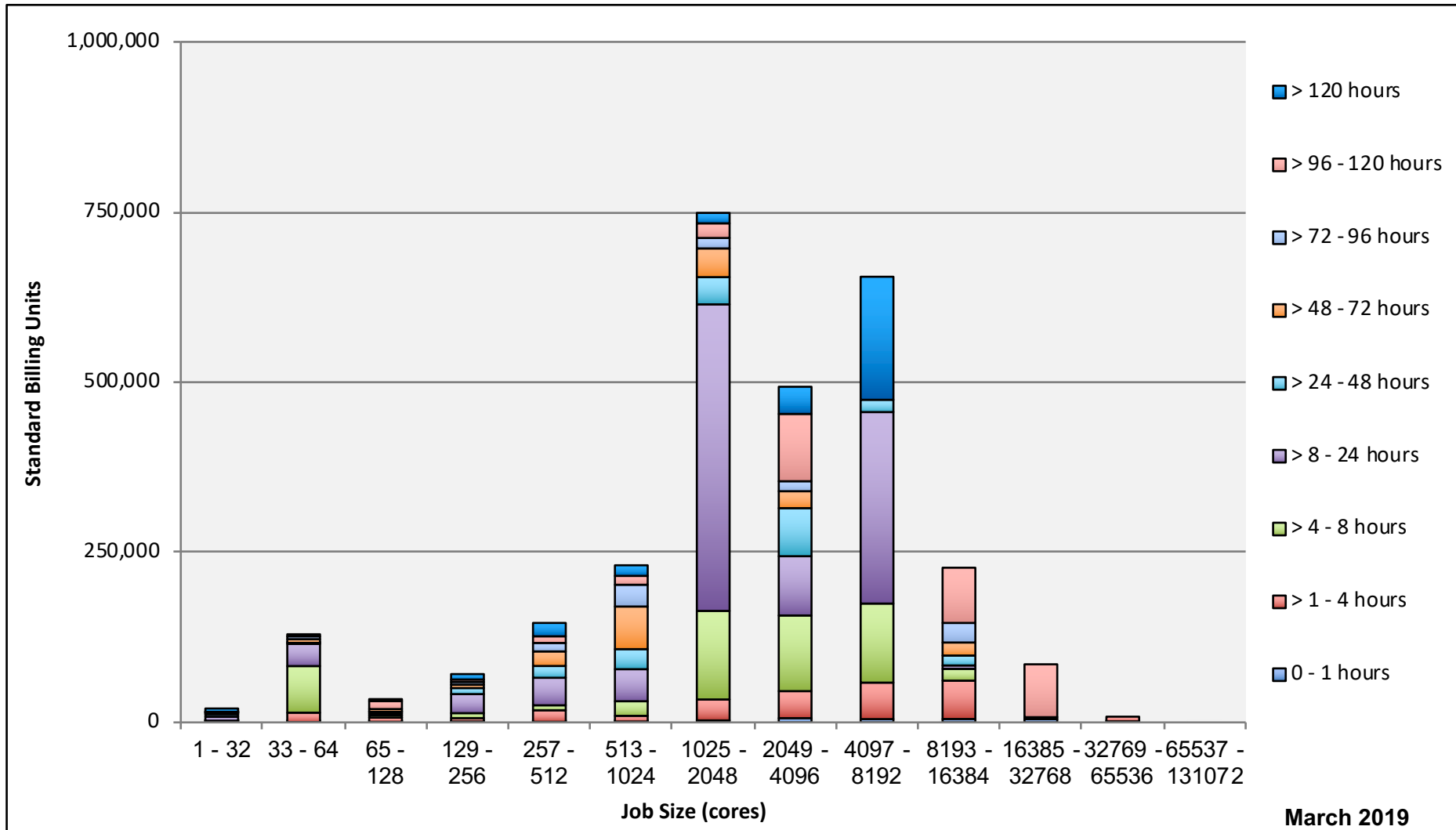
Electra: Monthly Utilization by Job Length



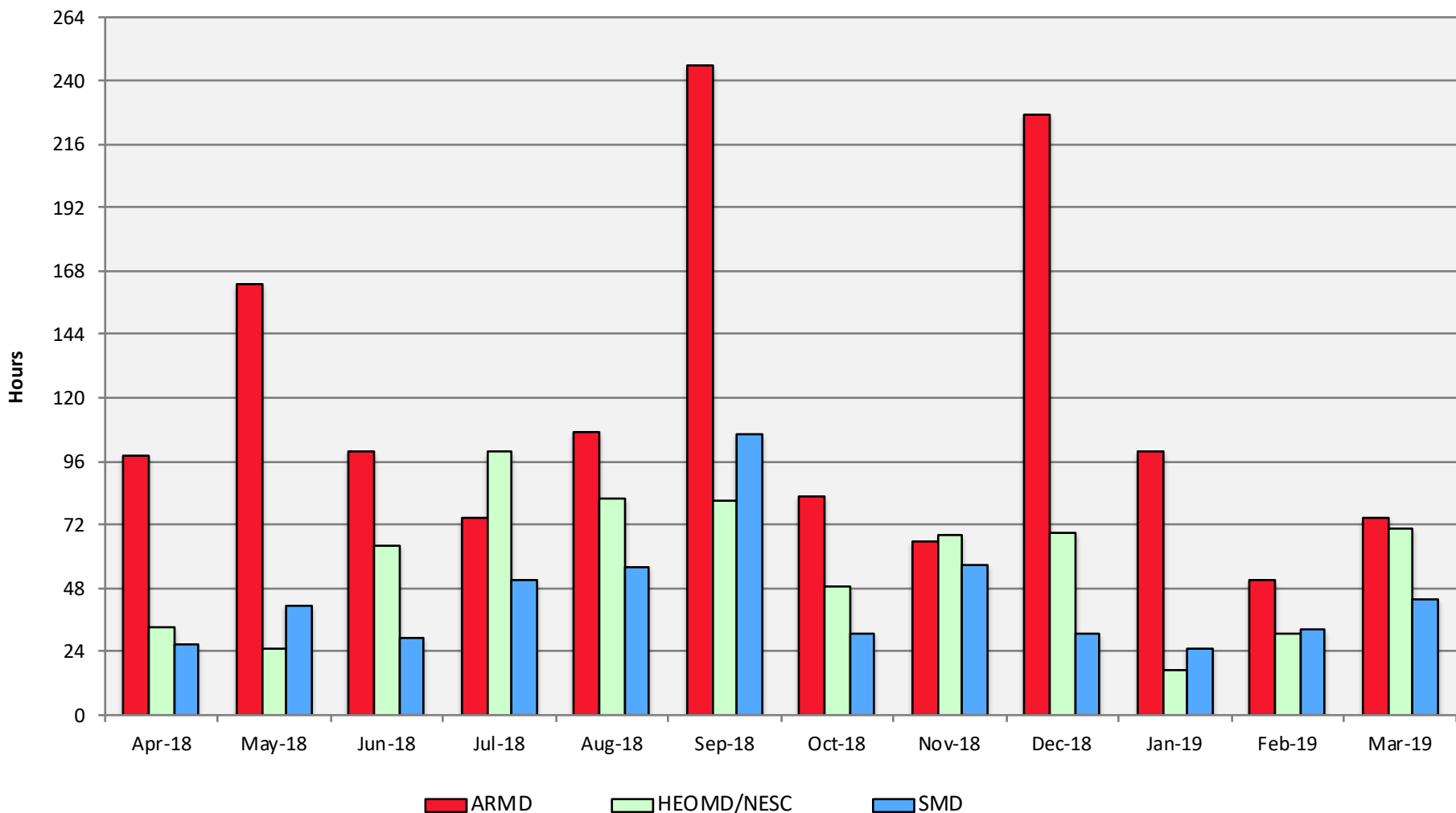
Electra: Monthly Utilization by Size and Mission



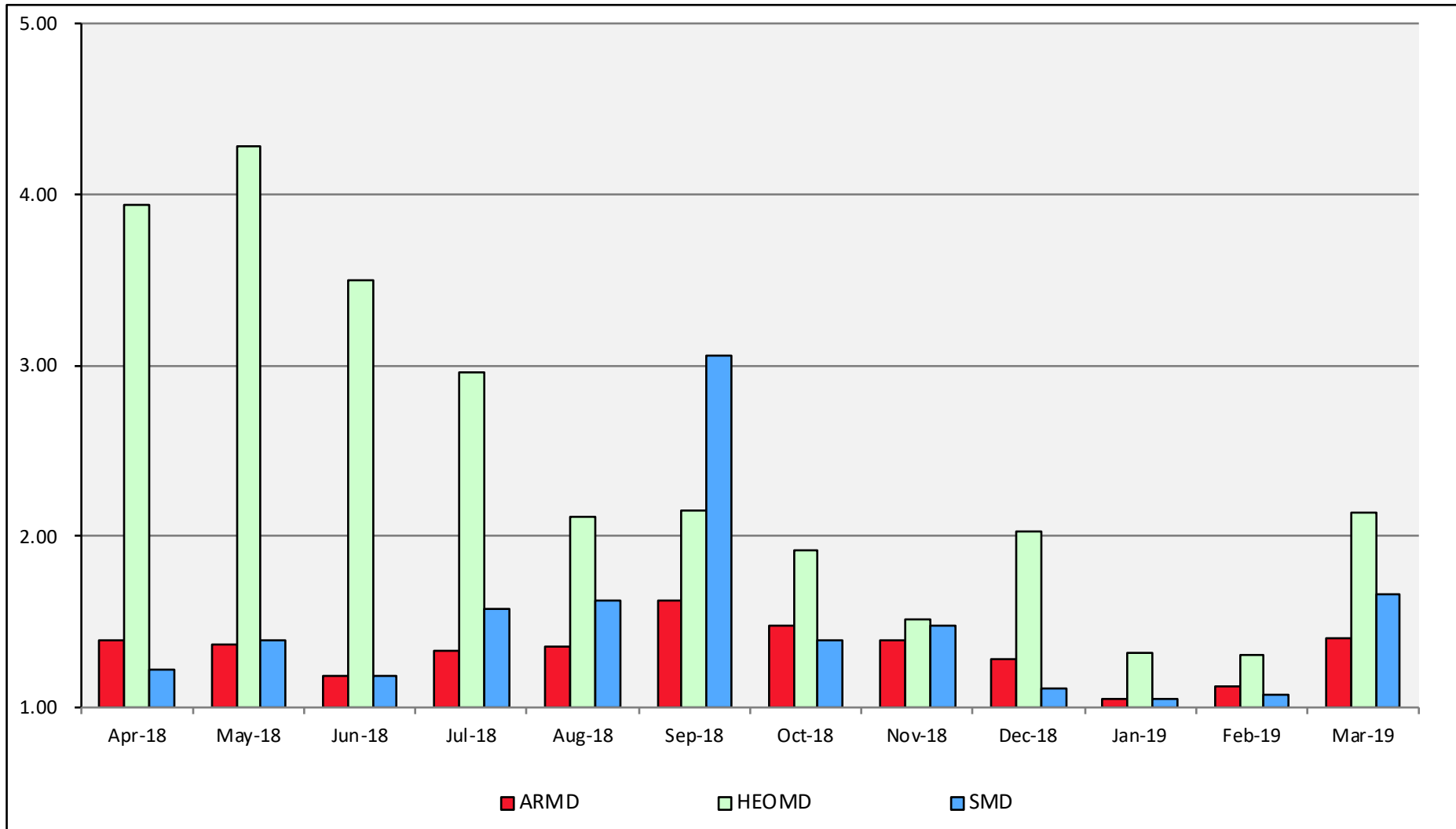
Electra: Monthly Utilization by Size and Length



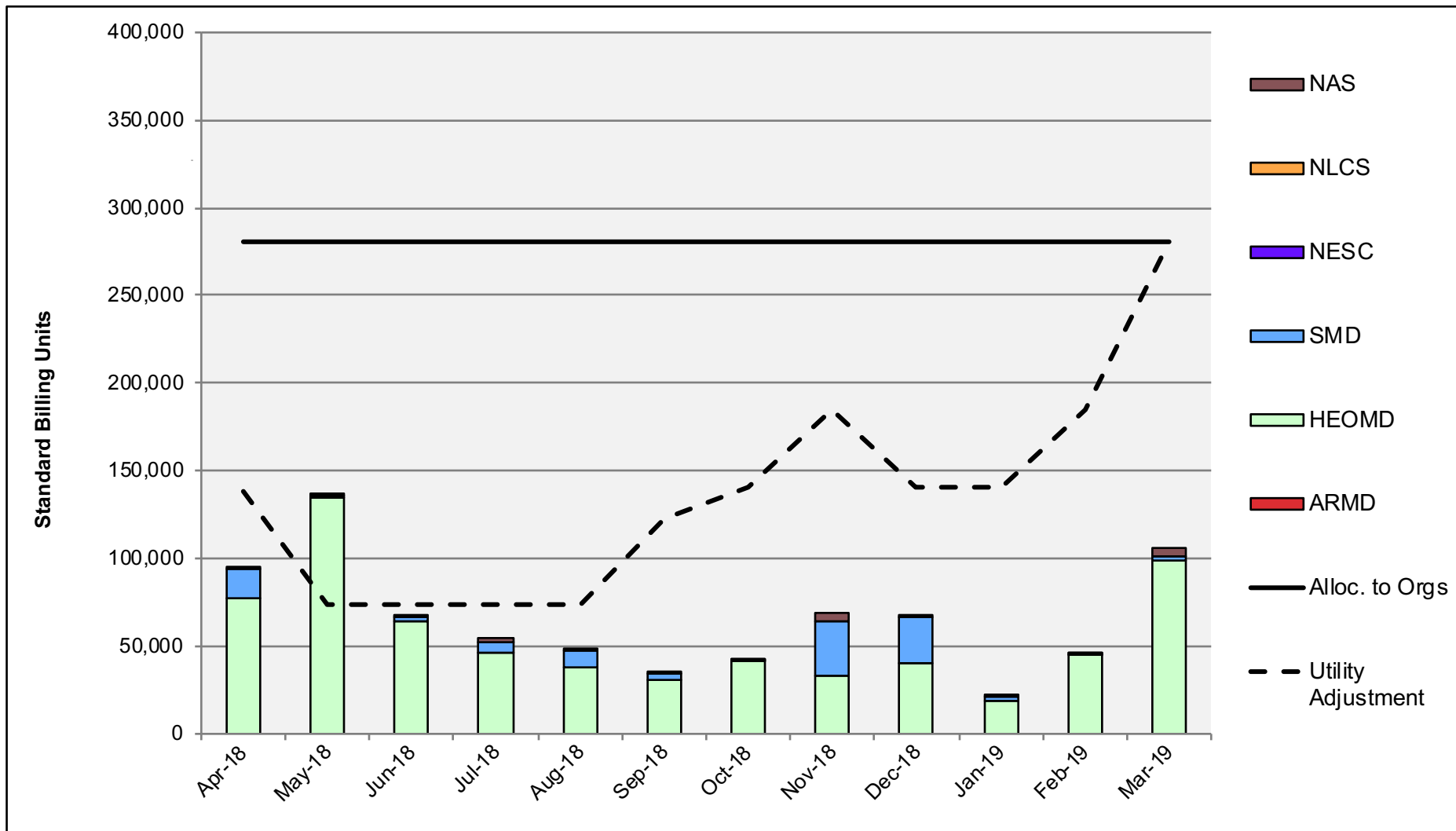
Electra: Average Time to Clear All Jobs



Electra: Average Expansion Factor

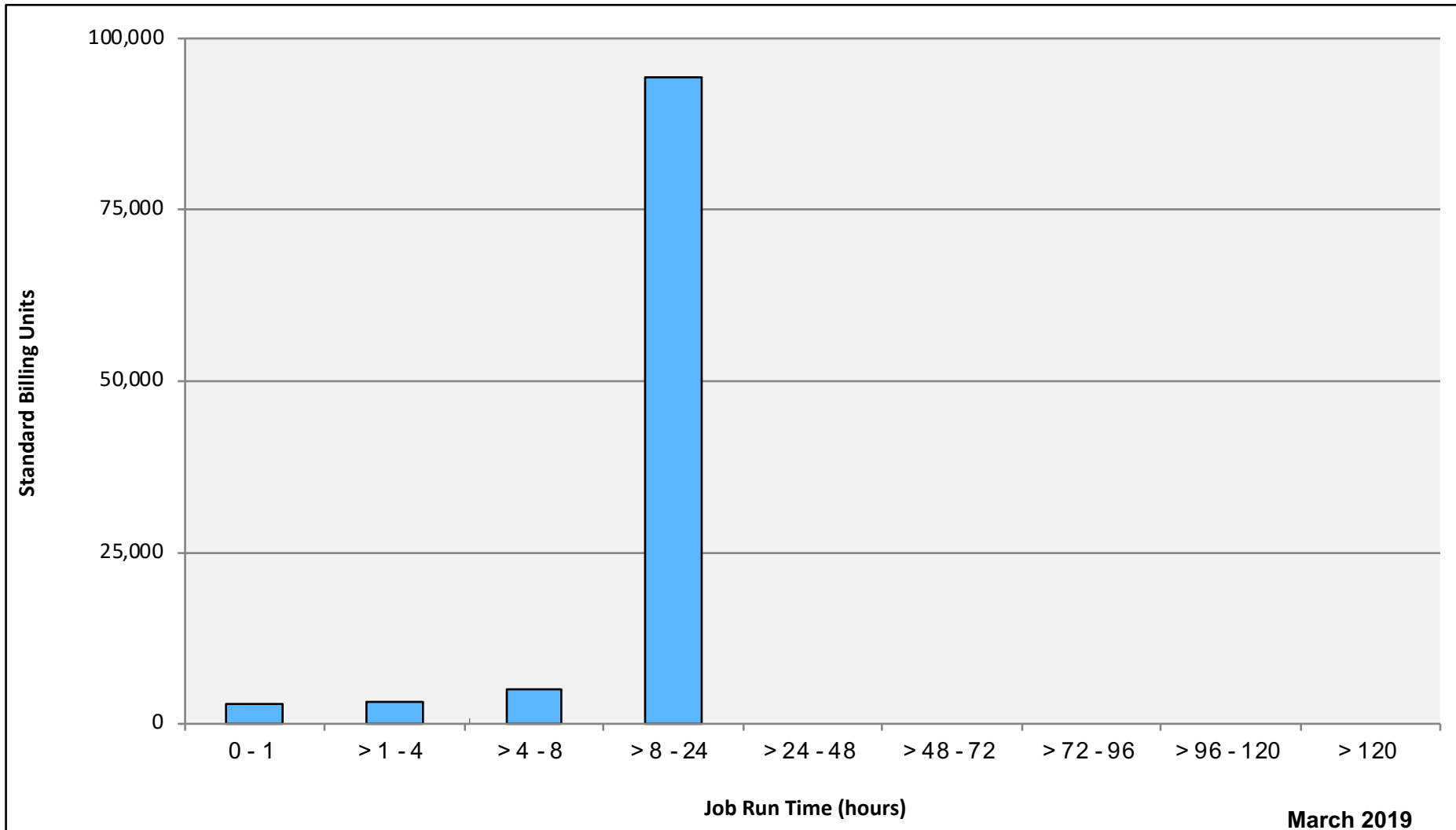


Merope: SBUs Reported, Normalized to 30-Day Month

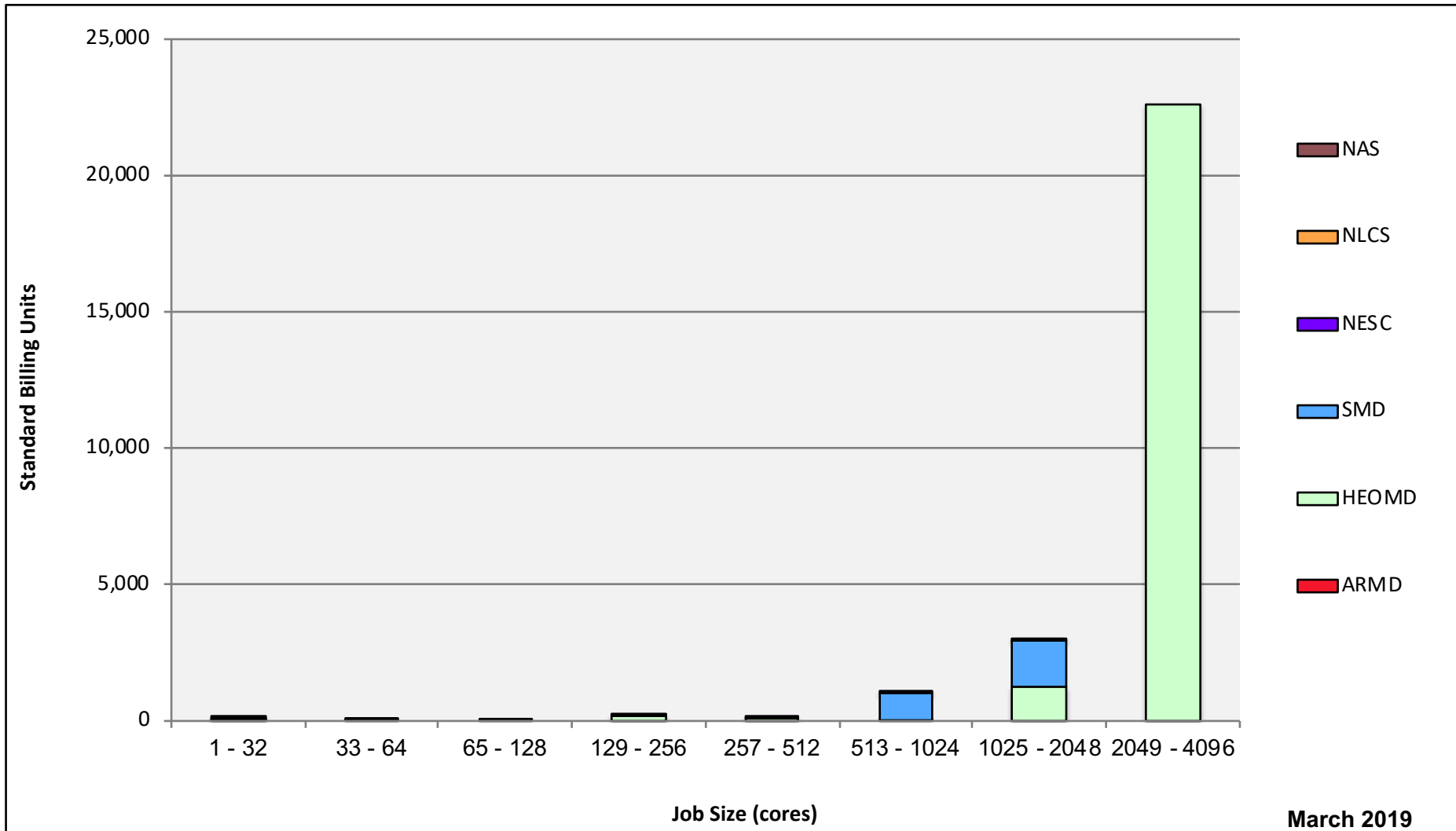


*Utility Adjustment: Multiple failures of chillers in N233A necessitated turning off a large portion of Merope

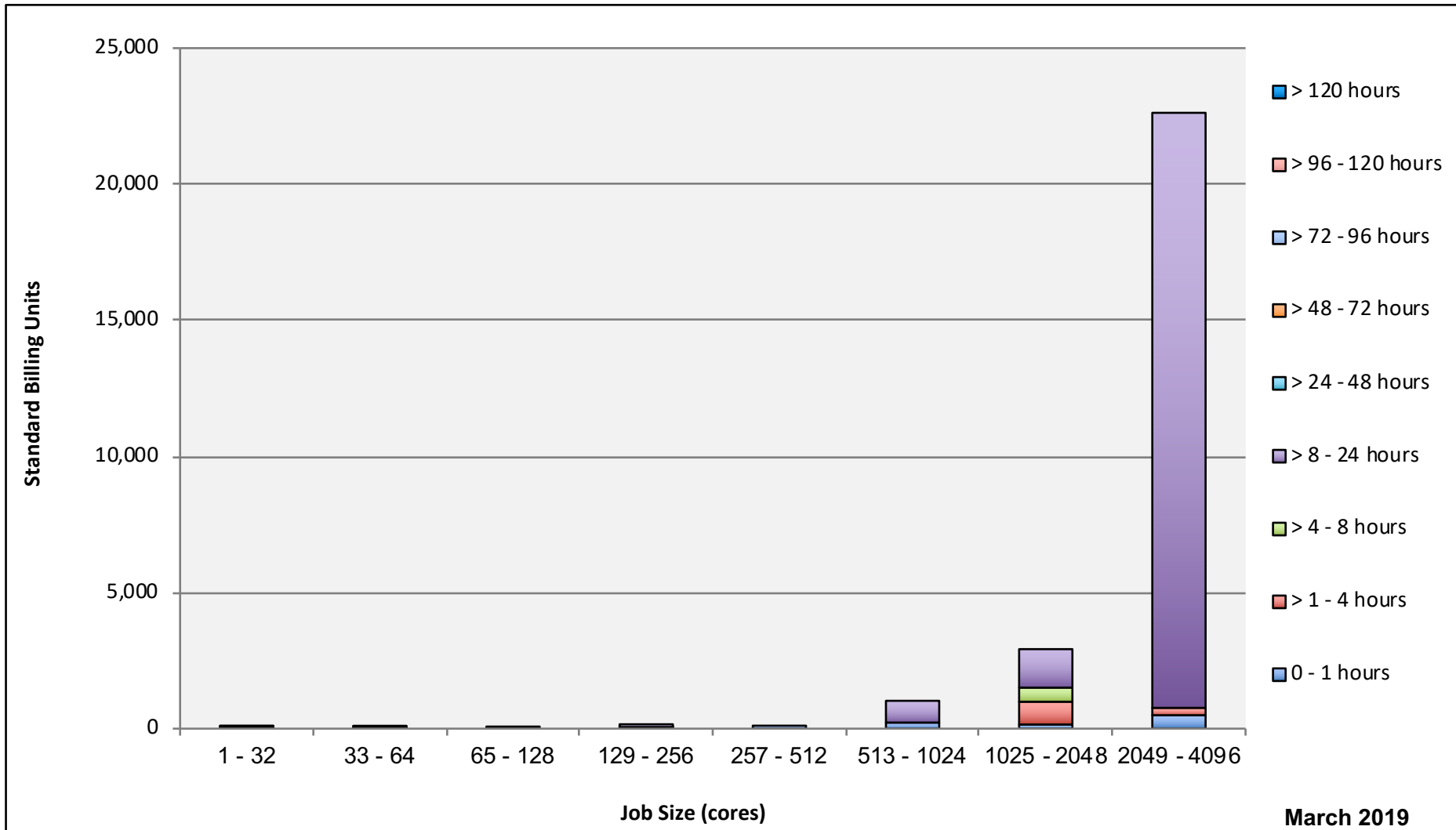
Merope: Monthly Utilization by Job Length



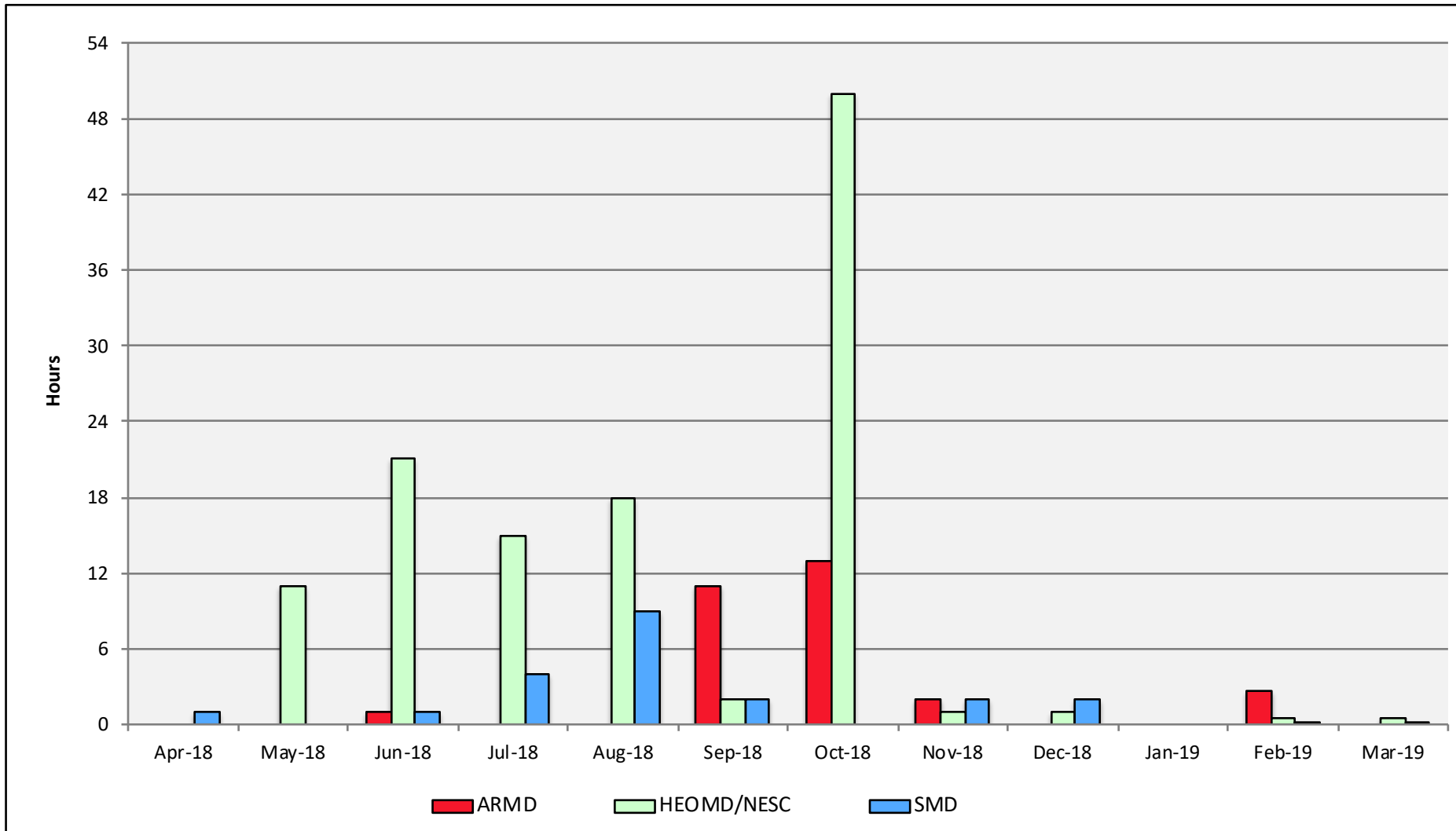
Merope: Monthly Utilization by Size and Mission



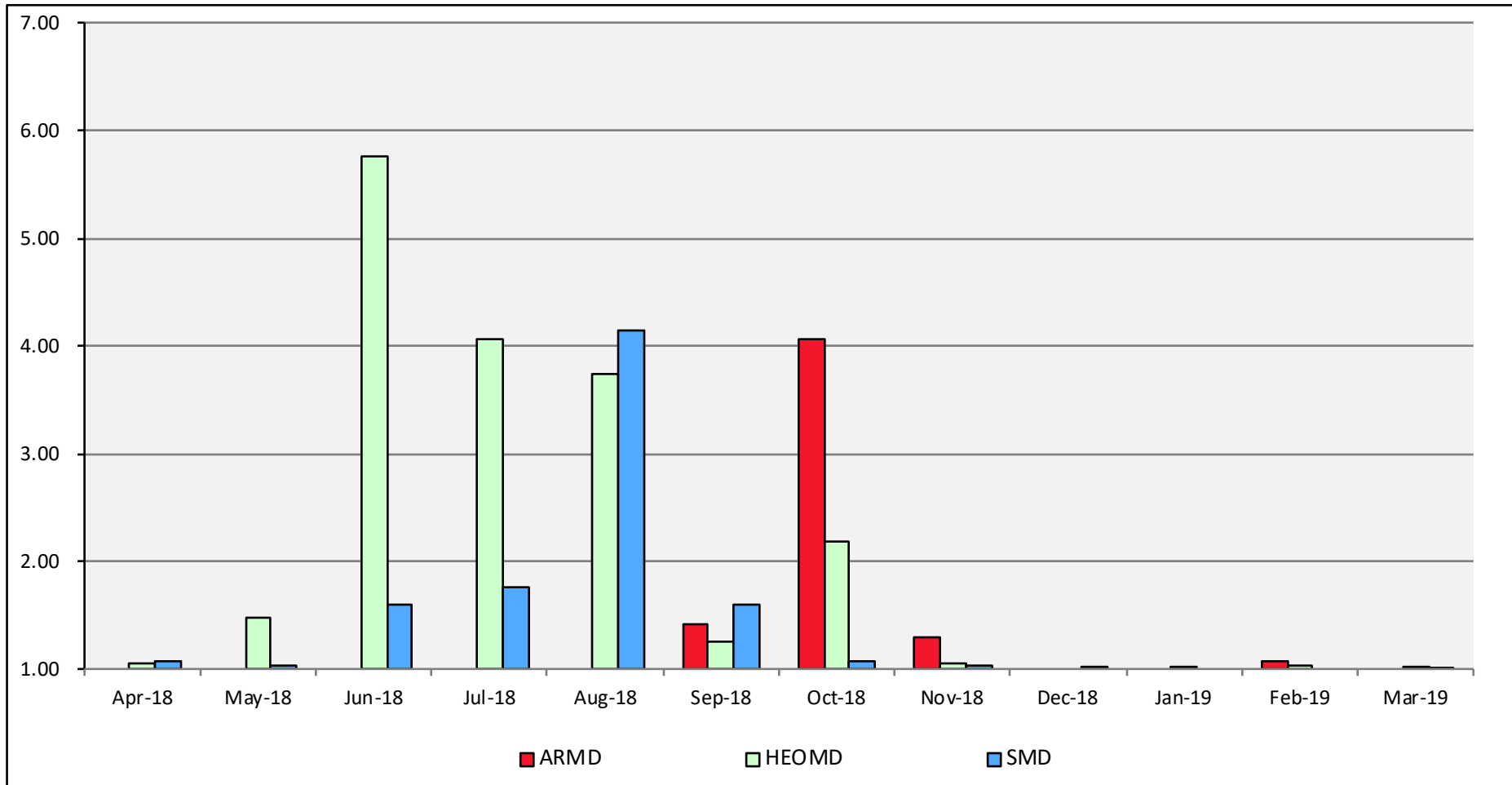
Merope: Monthly Utilization by Size and Length



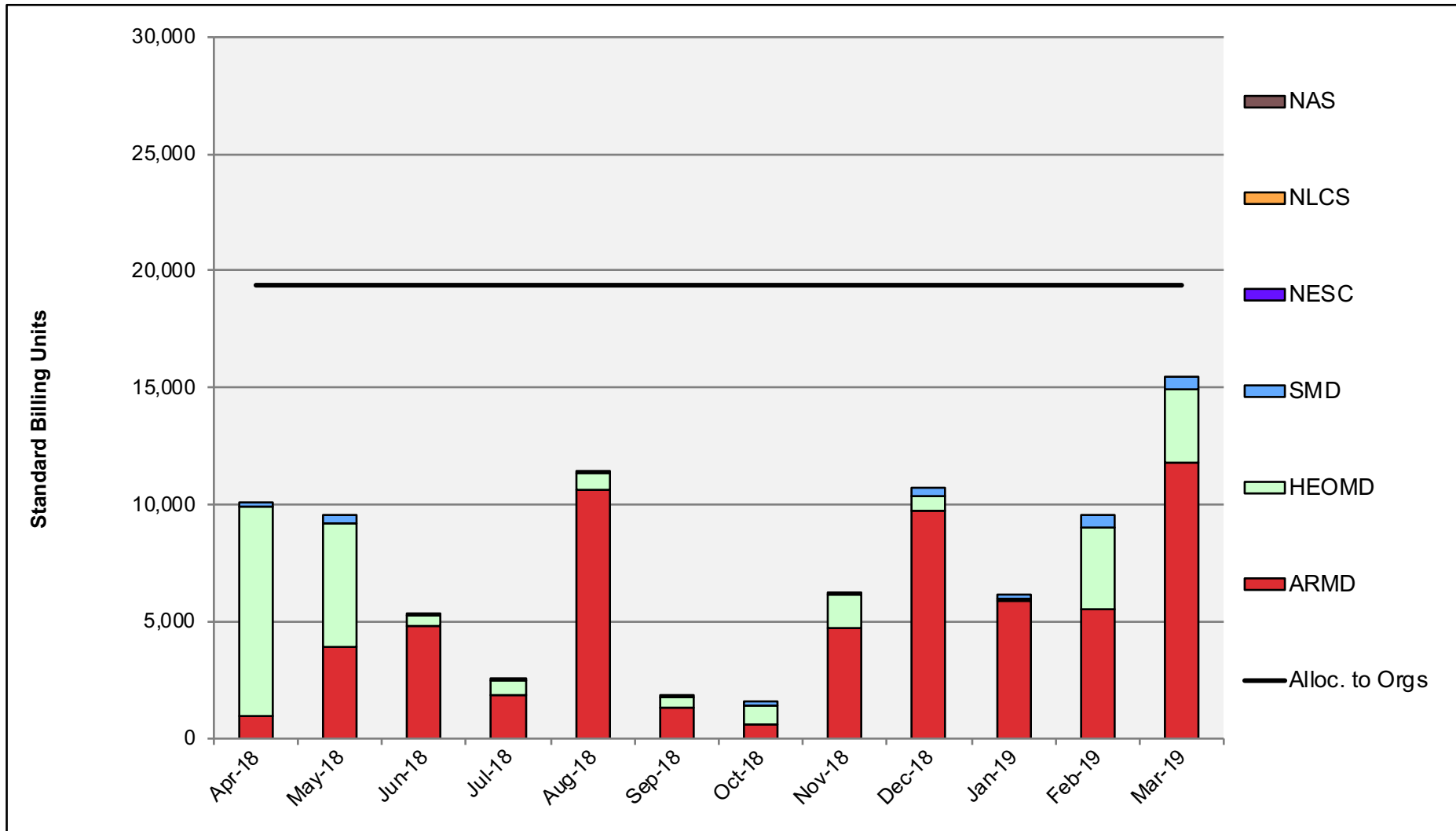
Merope: Average Time to Clear All Jobs



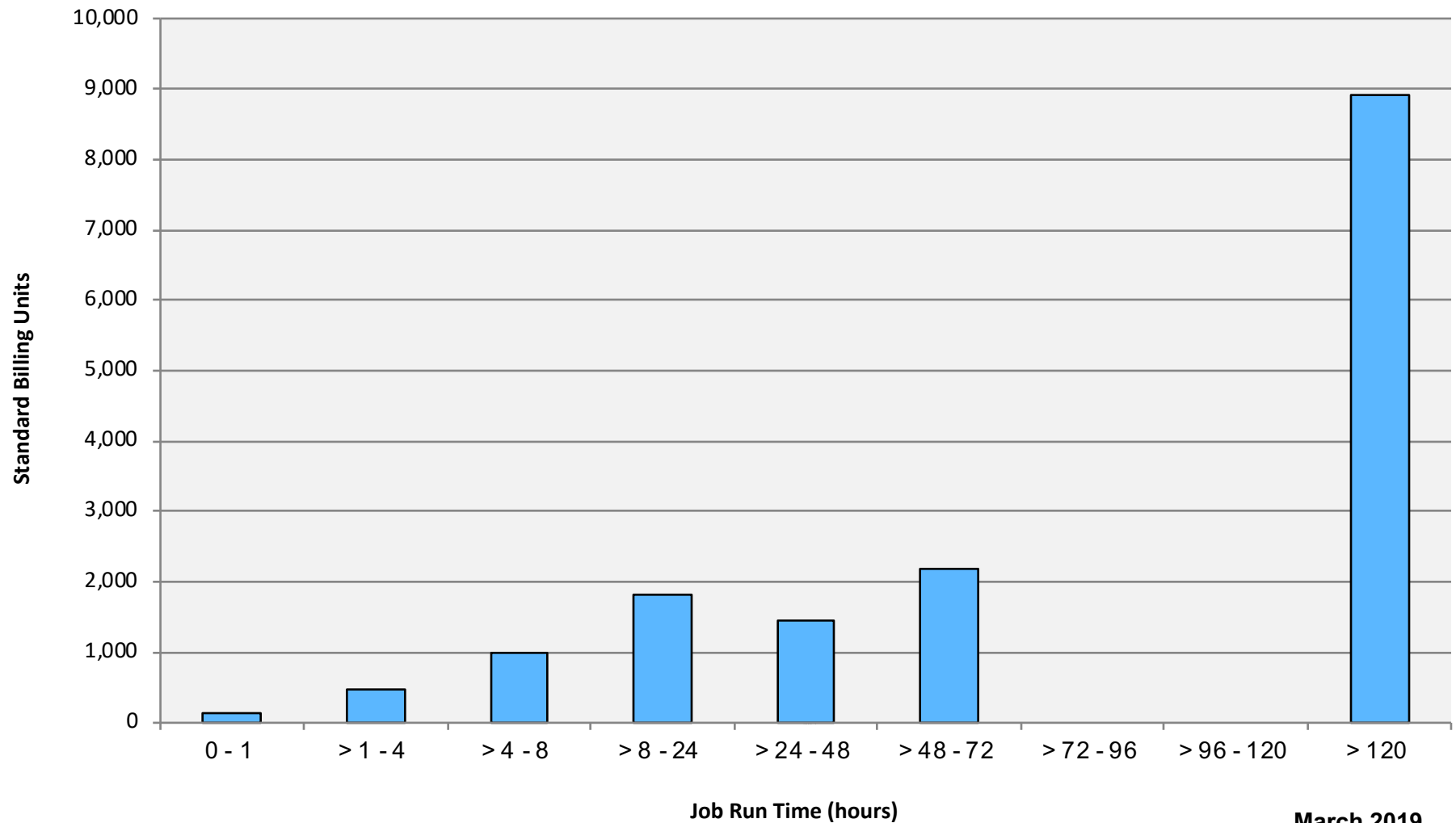
Merope: Average Expansion Factor



Endeavour: SBUs Reported, Normalized to 30-Day Month

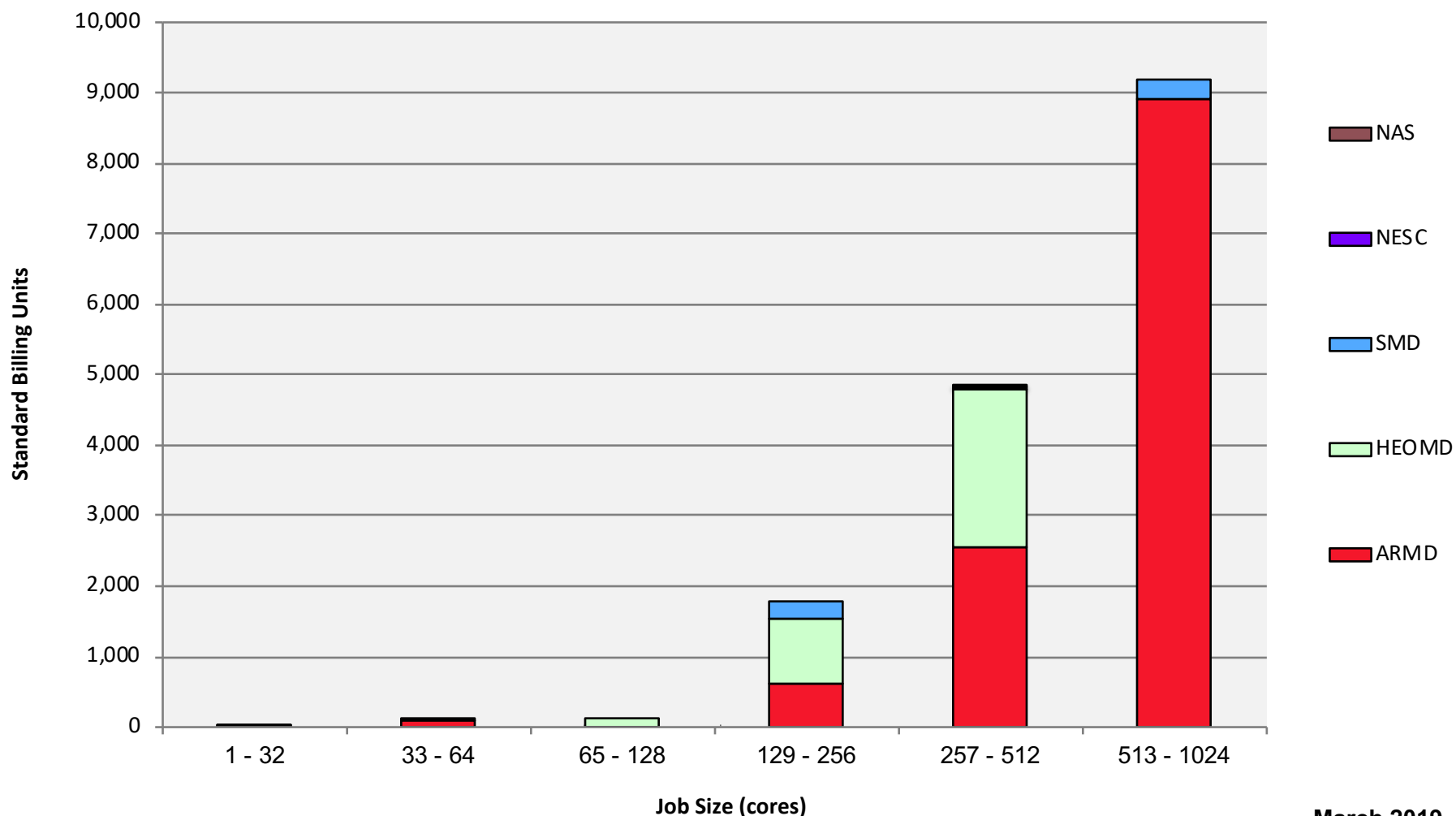


Endeavour: Monthly Utilization by Job Length



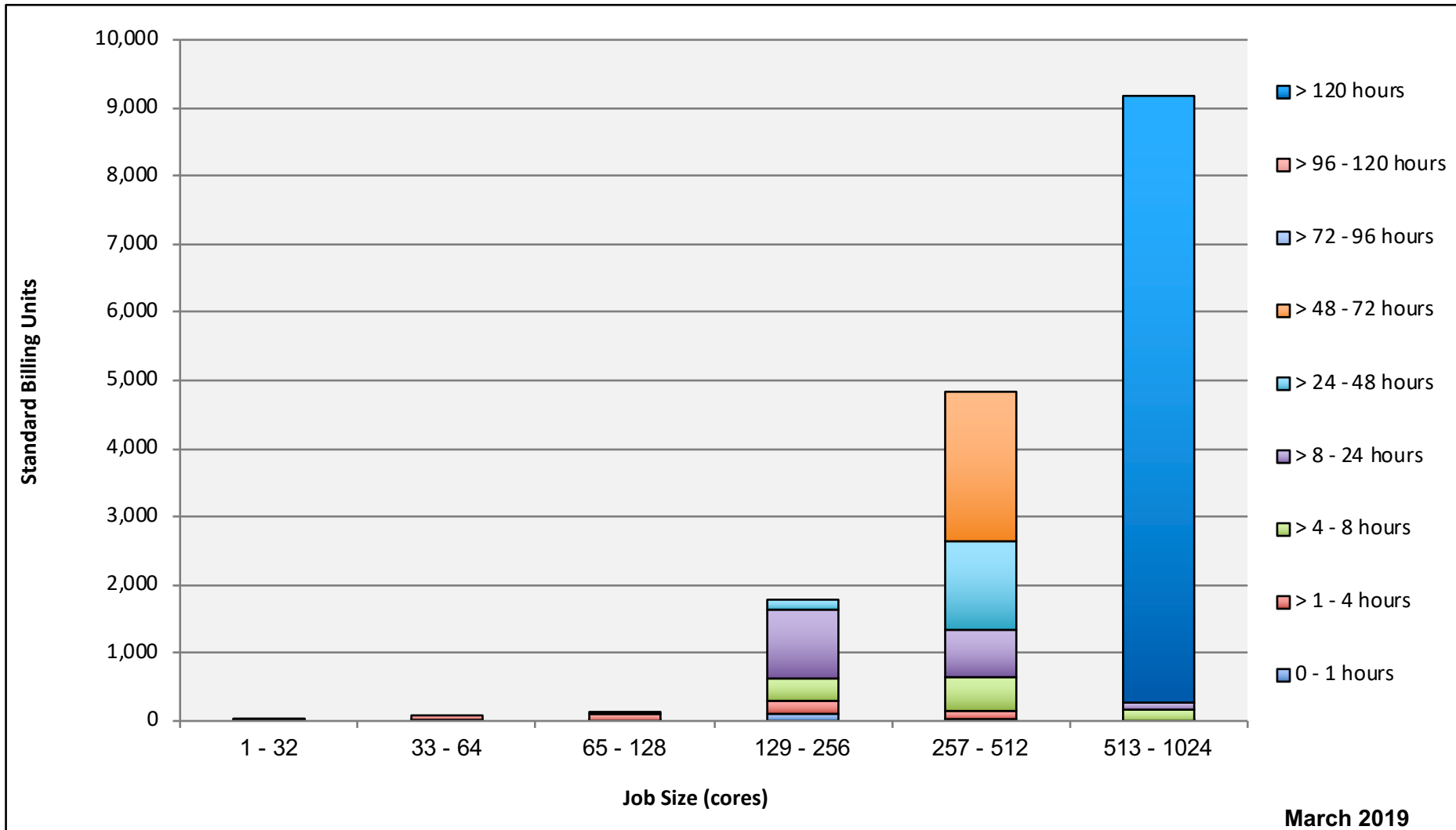
March 2019

Endeavour: Monthly Utilization by Size and Mission

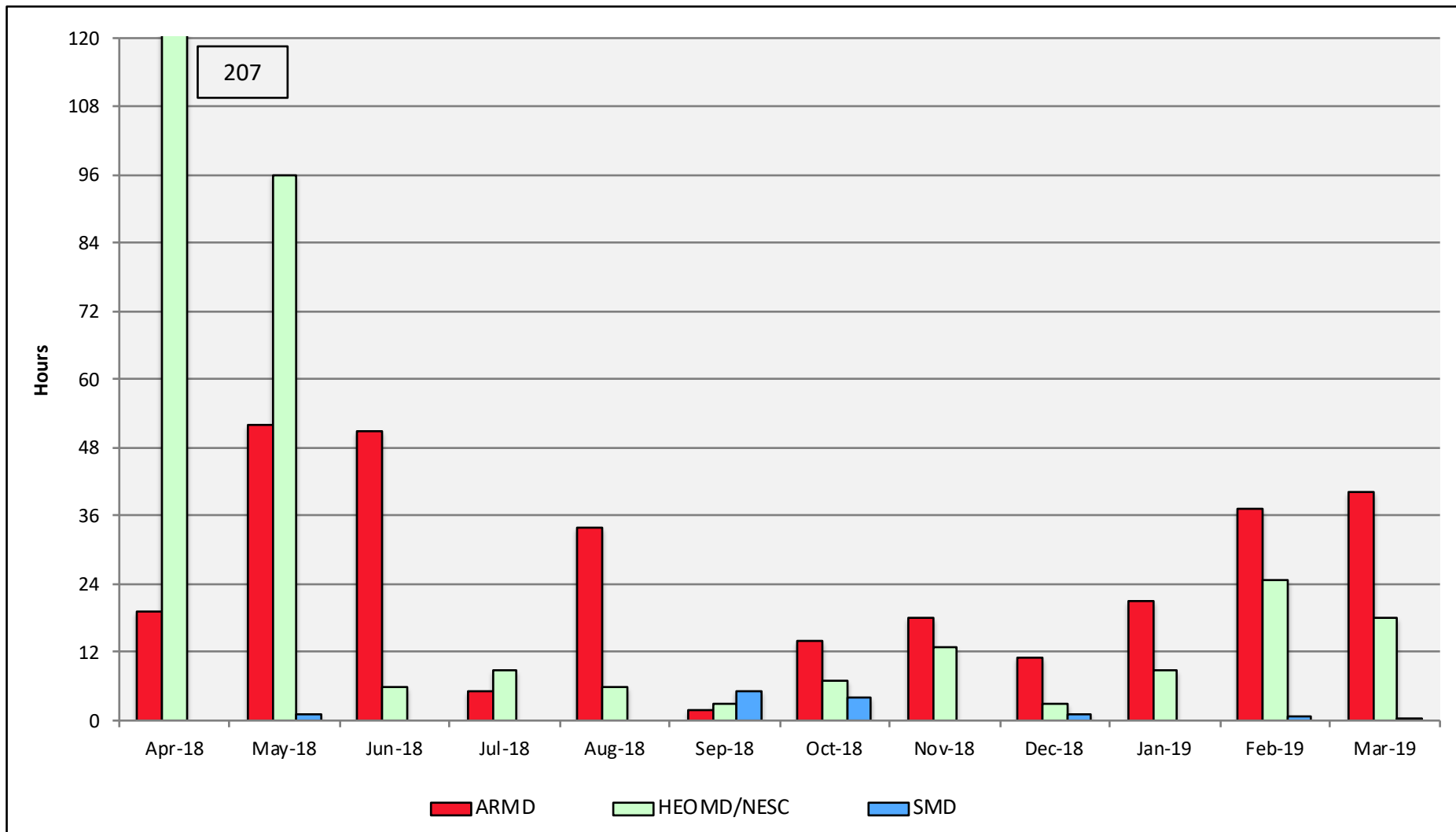


March 2019

Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor

